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CALCULATION OF THE LOWEST ENERGY STATE
OF THE CONDUCTION BAND OF GOLD

WALTER J. SLAZAK
and
FRANCESCO MUSORRAFITI

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Walter J. Slazak
and
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CONDUCTION BAND OF GOLD

by

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Submitted in partial fulfillment of
the requirements for the degree of

MASTER OF SCIENCE
IN
PHYSICS

United States Naval Postgraduate School
Monterey, California

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ABSTRACT

A new central field potential was developed for the metal gold by a variational technique in conjunction with the Wigner Seitz cellular method using the Control Data 1604 Computer to perform the calculations. The Hartree potential for the Au^+ ion was used as a starting point of the variations. The first variation was made fixing one point of the Hartree potential and letting the shape of the potential curve vary arbitrarily. The particular potential was chosen which furnished the lowest energy state solution to the Schroedinger radial wave equation subject to the boundary condition that the solution also furnished the proper ionization energy. A second variation was made varying the initially selected fixed point. This variation was terminated when the solution furnished the accepted value of the atomic radius, 1.59 Angstrom units. The results of the calculation indicate a lowest energy state of 1.194 Rydbergs and a cohesive energy of 81.6 kilogram calories per mole which compares favorably to the accepted value 83.5 kilogram calories per mole.

The wave functions from the developed potential indicate that the exchange interaction between the outer electrons are a major contribution to the cohesive energy.

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INTRODUCTION

The original scope of the thesis was to determine the lowest energy state of the conduction band of gold employing the cellular method, using a known tabulated potential.

The investigation progressed in five distinct phases.

The initial efforts were mainly along classic lines. A program was developed to use the Control Data 1604 Computer as a tool to make the computations. The initial results looked very promising. A method was devised to make a complete Wigner-Seitz (W-S) cellular calculation with one program. Work had begun to include correlation and exchange interactions. The Thomas Fermi potential was used in these initial investigations. The results for copper, even though they did not agree with the accepted values, seemed to agree with what had been done by others. Wave functions and W-S calculations were made for about twenty metals and carefully cataloged, with the aim that as the methods developed for gold the calculations could be repeated for other metals.

The second phase was a phase of great distress. By this time a very great number of calculations had been made and it was observed that the results were not consistent. Different intervals, changes of scale during calculation and different computational methods gave different results. At this point the exact cause of problem was unknown. Possible causes were estimated to be: improper programming, machine malfunctioning, input data too crude, inadequacy of numerical computational methods, or invalidity of the Wigner-Seitz cellular method. In any case except for an invalid program or improper machine operation, the problem area was one of far-reaching consequences. Standard computation methods had been used and

if these methods were at fault there would be implications that all computations to date were nonsense. If the cellular method did not converge, then too all the computations to date would have to be discarded.

The third phase was spent in isolating and resolving the problem area. This was accomplished in the following manner. The test vehicle used was the calculation of the wave functions of sodium as in the original Wigner-Seitz paper.¹ The potential used in this calculation was the Prokofiev ion core potential. This potential is represented by a series of parabolas, therefore there was no problem of fitting points to any interval. A unique method of solving the Schroedinger Differential Equation was devised based on an extension of Boole's Operational Methods.² In essence the method consisted of solving the entire problem in steps as a series of boundary value problems, requiring convergence at each step. The original Wigner-Seitz Data¹ was duplicated using this method. It was also found that a simple difference formula at one one-hundredth Bohr unit interval also duplicated the data. The results of the investigation confirmed the validity of the Wigner-Seitz method and provide a tool to continue the calculations. The investigation also indicated that predictor corrector type calculations in general as well as interval changes during a calculation led to erroneous results and were useless for this work. All previous work to this date had to be discarded.

¹E. Wigner and F. Seitz, Phys. Rev. 43, 804(1933) and Phys. Rev. 46, 509(1934).

²G. Boole, Treatise on Differential Equations, Supplementary Volume (The University Press, Cambridge, 1865) Chapter XXX.

The fourth phase was to use the method as developed on existing potentials of the noble metals. The results were disappointing and were not as good as the previous erroneous calculations. One striking physical fact was noted. When the method was applied to sodium using the ionization energy in the calculation the proper form of the wave functions resulted. All of the potentials of the noble metals investigated represented an ionization energy that was appreciably lower than the accepted value.

The fifth and final phase was used to develop a new metallic gold potential. The question was posed: could a variational technique be used to find a potential which gave the proper ionization energy and possibly give a lowest energy state? This idea was based on the assumption that such a potential would be more than a bare ion core potential, but would include exchange, correlation and proper electron screening constants. The calculation proved successful using the computation procedures already established as above. A potential was devised which gives in the Wigner-Seitz cellular calculation for gold the accepted values of the atomic radius and cohesive energy.

The Cohesive Energy

The cohesive energy³ is defined as "the difference between the energy of a crystal in the normal bound state at absolute zero of temperature, and the energy of the isolated atoms or molecules of which it is composed."

The cohesive energy is discussed first in order to introduce the total contributions to the energy of a solid. A rather complete list of contributions to the cohesive energy is quoted from Jaswon⁴

. the total electronic energy of a solid may be regarded as the sum of three distinct contributions:-

1. The energy associated with the ion-cores, viz.
 - (a) the self-energies of the ion-cores. This is independent of interatomic distance until the closed shells begin to overlap, and hence does not enter into the calculation of the equilibrium lattice parameter and compressibility;
 - (b) the Coulomb interaction of the ion-cores;
 - (c) the exchange interaction of the ion-cores. This is not important in the alkalis owing to the large clearance between the ions, but it assumes greater importance for the noble metals--especially in determining the elastic constants;
 - (d) the Van der Waals interaction energy of the ion-cores. This is taken to be negligible for all except molecular solids and graphite, but may be a contributory factor in the high cohesion of the transition elements.
2. The energy associated with the valence electrons, viz.
 - (a) the kinetic energy;
 - (b) the potential energy (with respect to the field of the ion-cores);
 - (c) the Coulomb self-potential;

³F. Seitz, The Modern Theory of Solids (McGraw Hill Book Co., Inc., New York, 1940), p. 375.

⁴M. A. Jaswon, The Theory of Cohesion (Interscience Publishers, Inc., New York, 1954), p.p. 156, 157.

- (d) the exchange interaction energy. This may be regarded as a correction to (c) operative for electrons of parallel spin;
 - (e) the correction to (c) for electrons of anti-parallel spin. This is not included in the mean value $\overline{H}$ of the Hamiltonian of the solid, and has to be estimated independently.
3. The interaction between the valence and ion core electrons, viz.
- (a) the Coulomb interaction. This has already been accounted for by 2(b);
 - (b) the exchange and correlation interactions.

The Cellular Method

The cellular method is discussed in great detail in many standard works in solid state physics. In this paper only those portions of the cellular method which pertain to the problem at hand will be discussed.

Consider a face centered cubic crystal and consider the construction of a cell obtained by choosing one ion core as a center and then passing planes perpendicular to and at the midpoint of the lines between the chosen ion center and all other nearest neighbors. The result is a polyhedron known as the "Wigner-Seitz Cell." This polyhedron to a first approximation may be considered a spherical cell.

For a face centered cubic crystal the radius of this approximating sphere can be calculated equating the volume of the cell per electron to volume of the lattice per electron.

$$\frac{4\pi r_0^3}{3} = \frac{A_0^3}{4} \quad r_0^3 = \frac{3A_0^3}{16\pi} \quad r_0 = A_0(3/16\pi)^{1/3}$$

$r_0 =$ radius of sphere

$A_0 =$ edge length of the fundamental cube of a cubic lattice

Values of r_0 are indicated in Table I for copper, silver, and gold.

The Wigner Seitz Cellular Approximation⁵

The original work was accomplished for metallic sodium and is reviewed in some detail; first, in that the method was used in this thesis, secondly, the results of the calculations for the metal dosium were unusually close to the accepted values, and thirdly there is a difference in interpretation as to the constitution of the potential used.

The argument is that the polyhedral cell can to a first approximation be replaced by a spherical cell. An ion core potential was considered inside the cell, with the condition this potential was spherically symmetric or could be averaged out to be spherically symmetric. The basic Schroedinger equation becomes a radial wave equation in this case in the form:

$$\left[-\frac{\hbar^2}{2m} \nabla^2 + V(r) \right] \psi(r) = E \psi(r)$$

introducing $\psi(r) = rR(r)$

the equation becomes

$$\frac{d^2 R(r)}{dr^2} - \frac{2m}{\hbar} [V(r) - E] R(r) = 0$$

Introducing natural units

$$1 \text{ Bohr radius} = .529 \text{ Angstrom Units} = a_0 = \frac{\hbar^2}{4\pi^2 m e^2}$$

$$1 \text{ Rydberg} = 13.5 \text{ electron volts} = \frac{e^2}{2a_0}$$

The equation becomes

$$\frac{d^2 R(r)}{dr^2} - [2 V(r) - E] R(r) = 0$$

with E in Rydbergs

r in Bohr radii

⁵E. Wigner and F. Seitz, Phys. Rev. 43, 804(1933)

TABLE I

Values of the Edge Length of the Fundamental Cube for Cubic Lattices (A_o) and the Atomic Radius (r_o) for Gold, Silver, and Copper.

	<u>Gold</u>	<u>Silver</u>	<u>Copper</u>
$A_o = {}^a(\text{Angstrom Units})$	4.070	4.078	3.609
$r_o = (\text{Angstrom Units})$	1.59	1.59	1.41
$r_o = (\text{Bohr Units})$	3.01	3.01	2.67

1 Bohr Unit = .529 Angstrom Unit

^aF. Seitz, The Modern Theory of Solids, op. cit. p. 6

The boundary condition inherent in the cellular method required by the periodicity of the lattice structure and symmetry is that the derivative of the wave function in the direction perpendicular to the symmetry planes will be zero when evaluated at the plane. When the polyhedron is approximated to a sphere the boundary condition becomes

$$\frac{d\psi(r)}{dr} = 0 \quad \text{OR} \quad \frac{\partial R(r)}{\partial r} = \frac{R(r)}{r} \quad \text{WHERE} \quad r R(r) = \psi(r)$$

It was further assumed that the electrons outside the cell boundary represented a free electron gas and that the average energy per electron could be represented by the Fermi energy

$$\epsilon_f(r_0) = \frac{3\hbar^2}{10m^2} \left(\frac{3N}{8\pi} \cdot \frac{3}{N4\pi r_0^3} \right)^{2/3} = \frac{2.21}{r_0^2} \text{ RYDBERGS}$$

$\hbar$ = Plancks constant

m = mass of the electron

N = number of electrons per unit volume

r_0 = atomic radius (or radius of cell)

The potential used in the calculation was the Prokofiev ion core potential for sodium.⁶ This choice of potential was fortuitous in many respects as follows:

1. The potential was obtained from actual data.
2. The potential was represented by a series of parabolas instead of just a number of points, thus the value of the potential at any value of could be determined accurately.

⁶E. V. Condon and G. H. Shortley, The Theory of Atomic Spectra (Cambridge University Press, London, 1951), p.343.

3. Within the first 1/100 interval, the potential is a constant. Therefore an initial power series expansion around the origin is valid. This initial power series expansion is required to furnish starting values for the wave function calculations by iterative processes.

The most important and striking feature of the potential is that when the radial wave equation is solved using the ionization energy for E , the resulting wave equations approach zero as r approaches infinity. Thus this potential actually represents the ionization energy and is physically much more than a simple ion core potential. Included within the potential are exchange, electron-electron and ion-ion contributions. This interpretation may be disagreed with on the grounds that non-central fields would be represented by central fields if the interpretation was correct. Actually the interpretation given implies that the contributions to the potential are smeared out in the spherical symmetry approximation. Also - since the results were close to the accepted values, it appears that there is more involved than the coincidence of various contributions cancelling each other. The contributions may actually be physically present in the potential. The results also indicate that the spherical symmetric model is a very good model for sodium.

The equation
$$\frac{d^2 R(r)}{dr^2} - 2 [V(r) - E] R(r) = 0$$

was solved for different values of the energy. Curve 1 of Fig. 1 represents the radial wave function when E is equal to the ionization energy. Curve 2 represents the radial wave function for a higher energy. The boundary condition $\frac{\partial R(r)}{\partial r} = \frac{R(r)}{r}$ is met at two points on Curve 2. This boundary condition is met only at one point on Curve 3, and not at all for higher values of E .

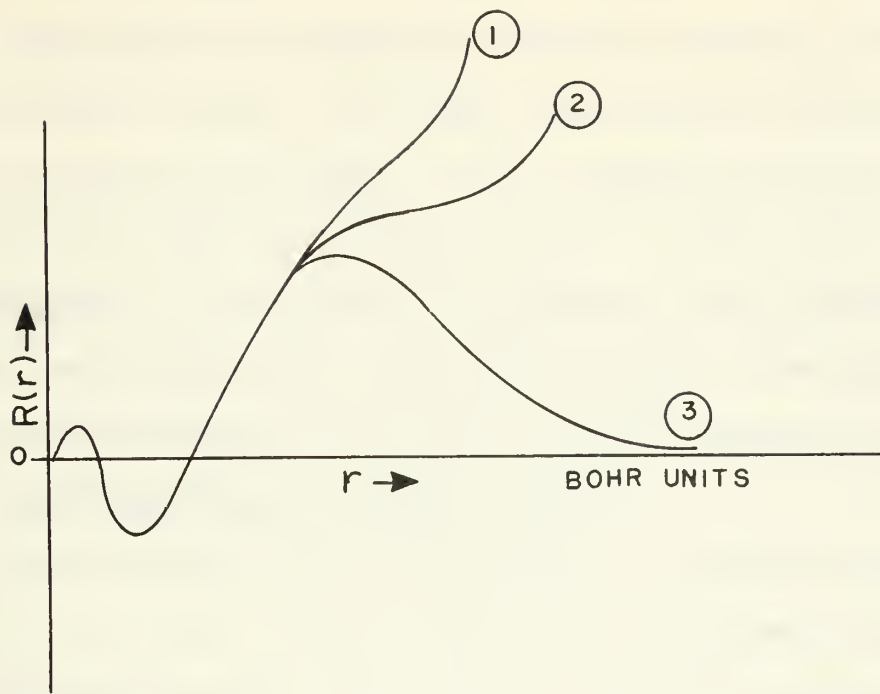


Fig. 1. Plot of the Radial Wave Functions $R(r)$ vs. Radial Distance (r) for a Wigner Seitz Cellular Calculation of a Metal. The wave function 1 represents the ionization energy. The wave function 3 represents the lowest energy state.

The values of E satisfying the boundary conditions are plotted vs. r as in Curve 1 in Fig. 2. The lowest energy state is that point determined by the curve with one tangent. Curve 2 represents the total energy and includes the addition of the Fermi energy for a free electron gas. The atomic radius, or the radius of the spherical cell is indicated by the lowest point on this curve. The cohesive energy is the difference between the ionization energy and the value of Curve 2 evaluated at r_0 .

The Thomas-Fermi Universal Potential^{7,8}

This potential which is represented by a tabulated function can be scaled to any value of Z the atomic number. The Thomas-Fermi potential is an approximate central field potential, obtained by treating a cluster of electrons around a nucleus by Fermi Dirac Statistics.

$$V(r) = \frac{Ze}{r} \phi(x)$$

$$r = bx$$

$$b = \frac{1}{2} \left(\frac{3\pi}{4} \right)^{2/3} \cdot \frac{a_0}{Z^{1/3}} = \frac{.88534 a_0}{Z^{1/3}}$$

$\phi(x)$ is a tabulated function

Z = atomic number

r = radius in Bohr units

a_0 = 1 Bohr radius = .529 Angstrom units

e = Charge on the electron

⁷H. J. Brudner, A Thomas-Fermi Technique for Determining Characteristics of Alkali Atoms with Excited Valence Electrons (New York University, College of Engineering, prepared for The Office of Naval Research, Physics Branch, Washington, D.C., 1959) and Accurate Thomas-Fermi Potential Distributions for the Alkali Ions (New York University, College of Engineering, Research Div., prepared for The Office of Naval Research, Physics Branch, Washington, D.C., 1959, Contract No. ONR 285(15)).

⁸E. V. Condon and G. H. Shortley, op. cit., p. 337.

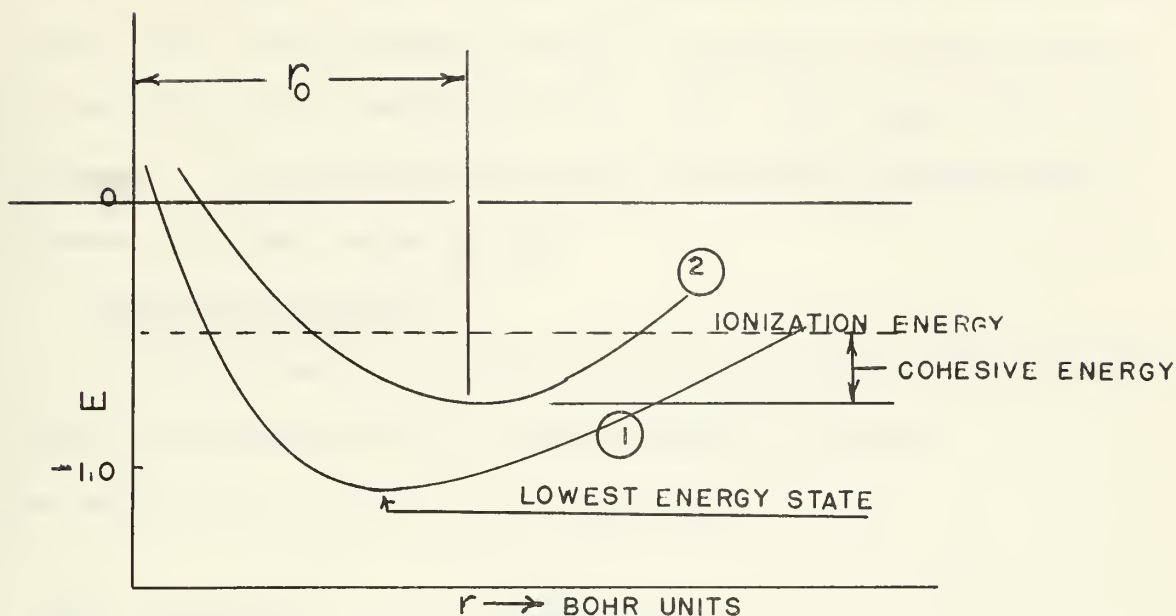


Fig. 2. Plot of the Energy (E in Rydbergs) vs. the Radial Distance (r in Bohr units) for Values of the Wave Function $R(r)$, Satisfying the Boundary Condition:

$$\frac{\partial R(r)}{\partial r} = \frac{R(r)}{r}$$

Curve 1 portrays the fundamental relation. The lowest value of energy on Curve 1 represents the lowest energy state. Curve 2 is obtained from Curve 1 by the addition of the Fermi Energy. The value of r at the minimum of Curve 2 represents the atomic radius. The energy difference between the ionization energy and the minimum of Curve 2 represents the cohesive energy.

A partial table of $\phi(X)$ for the free atom is found in Condon and Shortley.⁹ Brudner¹⁰ gives values of the Thomas-Fermi potential for the alkali ions. It was observed that the ion potential for the cesium ion corresponded to the free atom potential except near large values of the argument X . These functions are given at one-tenth intervals of the argument X and were easier to use.

The Hartree Potential

A brief discussion of the terms used in the Hartree self consistent field is described herein for equations without exchange.

The equation for the radial wave function is

$$\frac{d^2 R}{dr^2} = 2 \frac{Y(n, \ell, r)}{r} - \epsilon_{n, \ell} - \frac{\ell(\ell+1)}{r^2} P(n, \ell, r) = 0$$

$\frac{Y(n, \ell, r)}{r}$ is the potential of the field of the nucleus and of the average distribution of the electrons.

$P(n, \ell, r)$ is the radial wave function, n, ℓ is a description of the state.

The field at radius r due to the charge on the nucleus and the average distribution of the electrons is $\frac{Z(r)}{r^2}$

$Z(r)$ is related to $Y(r)$ by the relations

$$\begin{aligned} \frac{dY(r)}{dr} &= \frac{1}{r} [Y(r) - Z(r)] \\ \text{or } \frac{d}{dr} \left[\frac{Y(r)}{r} \right] &= -\frac{Z(r)}{r^2} \end{aligned}$$

⁹E. V. Condon and G. H. Shortley, op. cit.

¹⁰H. J. Brudner, op, cit.

In the case of silver,¹¹ the values of $Y(r)$ are tabulated. In the cases of copper¹² and gold,¹³ the contributions to $Z(r)$ are given and $Y(r)$ is calculated by use of the above equations.

¹¹M. M. Black, *Memoirs and Proceedings of the Manchester Lit. and Phil. Soc.*, v. 79, 1934-35.

¹²D. R. Hartree, *Proc. Roy. Soc., London*, A 141,282 (1933).

¹³A. S. Douglas and D. R. Hartree, *Proc. Roy. Soc., London* (1934).

CALCULATION

The Initial Approach

The initial approach used the Thomas-Fermi potential in the calculation. The aim of the initial approach was to establish the program for the Control Data 1604 Computer to give results from which graphs like Fig. 1 and Fig. 2 could be plotted.

In dimensionless form the radial wave equation took the form

$$\frac{d^2 R}{dx^2} + \left[1.7706 Z^{2/3} \frac{\phi(x)}{x} - \frac{1.571 E}{Z^{2/3}} \right] R = 0$$

Z is the atomic number

E is the energy in units of two Rydbergs

$\phi(x)$ is the Thomas-Fermi tabulated function

A simple difference equation solution was adopted¹⁴ as follows:

$$\text{Let } f(x) = 1.7706 Z^{2/3} \frac{\phi(x)}{x} - \frac{1.571 E}{Z^{2/3}}$$

$$R(x + \Delta x) = \left\{ 2 - (\Delta x)^2 f(x) \right\} R(x) - R(x - \Delta x)$$

The program was successfully developed. A format was established using r in Bohr units as independent variable instead of x . In this format a contribution to the effective potential normalized to $1/Z$ could be inserted on data cards, changing only Z and the ionization energy for different elements.

$$\text{That is } V(r) = \frac{Z \phi(r)}{r}$$

¹⁴J. C. Slater, Mechanics (McGraw Hill Book Co., Inc., 1947), Appendix I.

Difficulties Experienced

In order to insure the most accurate calculation having established the format of the program, iterative methods reputed to be more accurate than the initial simple iterative formula were tried. The Milne¹⁵ fifth and seventh degree polynomial methods for second degree differential equations without a first order term were representative of accurate predictor-corrector type formulae.

It was observed that using the same potential that different numerical formulae gave different solutions. It was also noted that changing scale, or changing intervals during the course of the solution also gave different results.

Another major problem area developed, how to interpolate data. Much of the tabulated data is given to only two decimal places. This type of data to a machine that sees 12-100 decimal places appears as a widely scattered set of points. That is, the problem area was how sensitive are the various iterative formulae to crude data.

The basic form of the equation

$$\frac{d^2 R}{dr^2} = f(r) \cdot R$$

tends to become unstable¹⁶ for large values of r . The question arose, did spurious solutions which were originally eliminated by the boundary conditions creep back during the calculation?

¹⁵W. E. Milne, Numerical Calculus (Princeton University Press, 1949), p.p. 140-143.

¹⁶L. Fox, Numerical Solutions of Ordinary and Partial Differential Equations (Addison-Wesley Publishing Co., Inc., London, 1962) p.p. 46-57.

Investigation of the Problem Areas

The next basic step was to determine if the Wigner Seitz method was actually convergent, and if so, what scheme of calculation was required with the tools on hand to give a proper solution.

The vehicle for the investigation was the use of the Prokofiev potential to make a calculation for E equal to .5 Rydbergs. A plot of this function was available in the literature.¹⁷ At this energy there were two tangents to the curve. Since the Prokofiev potential is a series of parabolas the values of the function are readily calculated to any desired degree of accuracy by the computer. This potential eliminated one variable, scatter in the data.

The interval chosen was $1/100$ of a Bohr radius. Choosing a fixed interval eliminated another variable.

A new scheme was developed to solve the basic equation based on Boole's operational methods.¹⁸ A sketch of the method follows; full details are in Appendix I.

The first three points of the potential are approximated by a parabola. The radial wave equation is then solved in the interval of these three points. The value of the function and the derivative are then evaluated at midrange. The process is then repeated for the second, third, and fourth points, using the previous calculated values of the function and derivative as initial conditions. Thus in the range of 830 points the

¹⁷ E. Wigner and F. Seitz, Phys. Rev. 43, 804 (1933)

¹⁸ G. Boole, Treatise on Differential Equations, Supplementary Volume (The University Press, Cambridge, 1865), Chapter XXX

process is simply the solution of 829 boundary value problems. The solution turned out to be a very complex series solution, which converged at every interval. The length and complexity of the solution were initially disappointing in that one run required approximately twenty minutes of machine time, and would require a lifetime for one man to accomplish by ordinary calculation processes.

The Resolution of the Problem

The second derivative of $R(r)$ can be determined by two methods from the solution $R(r)$ as follows:

1. $\frac{d^2R}{dr^2} = f(r) \cdot R(r)$ the original equation.

2. Differentiate the function $R(r)$ twice with respect to r .

The values of the second derivative calculated by both of the above methods must match for the equations to be consistent.

The Radial Wave Functions $R(r)$ were calculated for sodium for the energy state, $E = 0.5$ Rydbergs by a variety of computational techniques including the boundary value method, the simple type difference method, and predictor-corrector methods.

The wave functions were then compared with the Wigner-Seitz wave function with surprising results. A summary of the results follows:

1. The boundary value technique proved successful. The values of the two second derivatives matched within 10^{-8} . The wave function matched the Wigner-Seitz function from the literature point by point.

2. The simple system after some small initial perturbations matched the solution calculated by the boundary value method within 10^{-6} for the function, the first derivative and the second derivative.

3. The predictor-corrector formulae gave varied results and did not

duplicate the Wigner-Seitz wave function. It was observed that this method of solution in matching the second derivative and holding the function could not hold the first derivative. The net result is that the first derivative was not continuous from point to point. The second derivative obtained by differentiating the first derivative turned out to be a series of widely varying oscillations.

4. In Fig. 3 the wave function calculated by the boundary value method and the simple method coincide with the wave function from the literature. The predictor-corrector method carried to three decimal places (duplicating hand calculation) differed greatly from the same method carried to five or one hundred decimal places.

The Criteria Established

The following criteria were established as a result of the investigation:

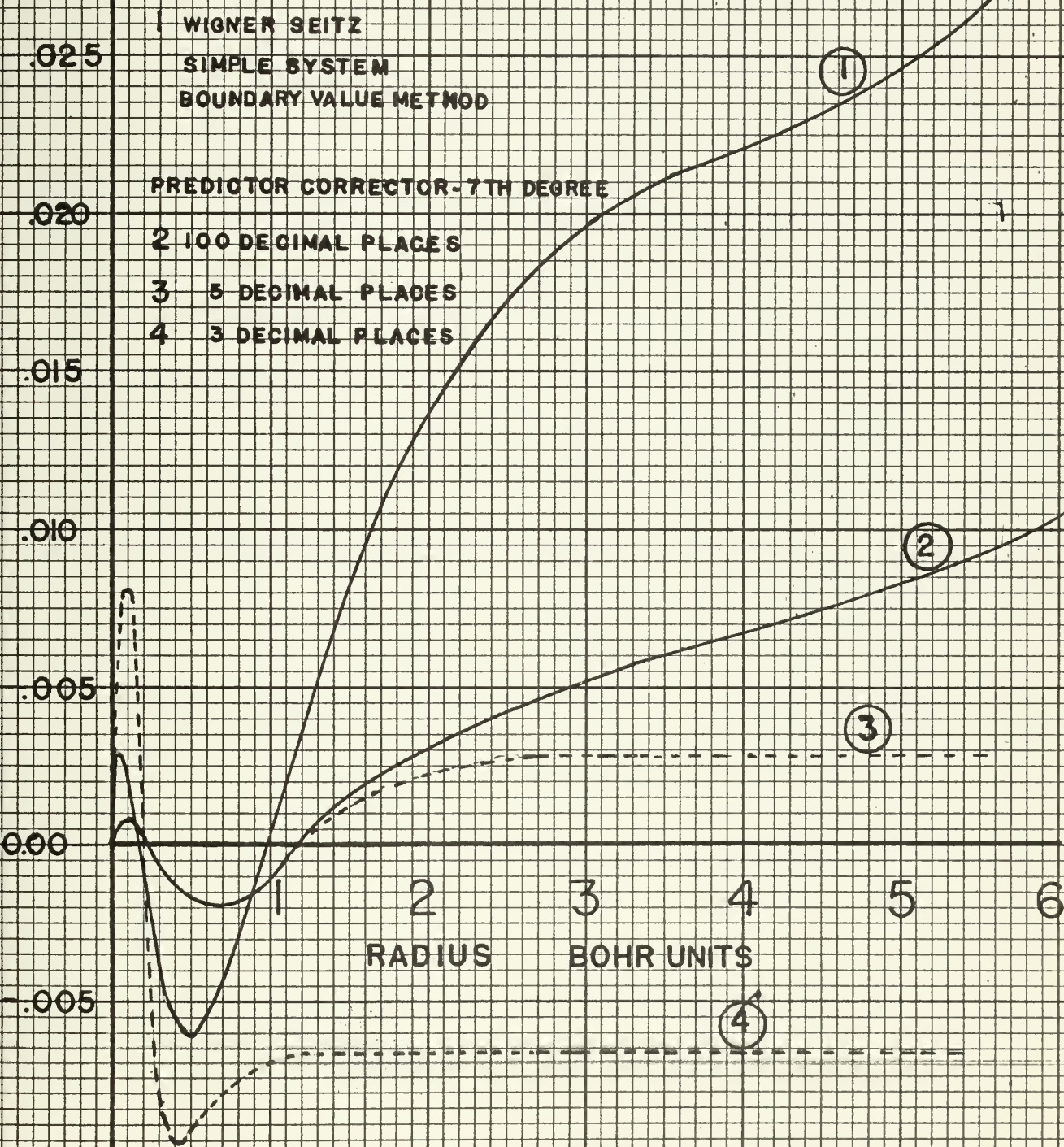
1. The simple method was adopted using the 1/100 Bohr Unit interval without any change in scale during the calculation.
2. The boundary value method would be used to obtain accurate starting values for the simple method.
3. Extreme care would have to be exercised in the data points used. The potential curves used were expanded graphically to insure that spurious "wiggles" were not introduced.

Conclusions

The problem had been resolved and it was concluded.

1. The Wigner-Seitz cellular method does converge, but much care must be used in the calculations as the many pitfalls along the way can lead to erroneous results which are not obviously erroneous.

FIGURE - 3 -
COMPARISON OF CALCULATIONS
FOR
THE RADIAL WAVE FUNCTIONS $R(r)$
SODIUM $E=5$ RYDBERGS



2. The calculations would be carried out using the above mentioned criteria without further refinement.

WIGNER-SEITZ CALCULATIONS FOR THE
NOBLE METALS USING EXISTING POTENTIALS

The Potentials Used

The Hartree silver potential¹⁹ and the Thomas-Fermi potential are compared in Fig. 4 on a log-log plot. It is observed there is rather close agreement between the two potentials. The Thomas-Fermi free atom potential was arbitrarily fitted into the Hartree potential for large values of r so that the Thomas-Fermi potential would resemble an ion core potential.

The Hartree Fock copper potential²⁰ and the Thomas-Fermi copper potential are compared on a log-log plot in Fig. 5. The Hartree potential is not shown as it agrees fairly well with the Thomas-Fermi potential.

The Hartree gold potential²¹ and the Thomas-Fermi gold potential are compared on a log-log plot in Fig. 6. It is again noted that there is rather good agreement.

The wave functions for the noble metals employing the six potentials discussed above are graphically portrayed in Figs. 29 through 75 (See Appendix II) for the range of energies varying from the ionization energy to the lowest energy state. These graphs are depicted as obtained from the computer graph routine without retouching.

¹⁹ M. M. Black, op. cit.

²⁰ G. W. Pratt, Phys. Rev., 88, 1217 (1952).

²¹ A. S. Douglas and D. R. Hartree, op. cit.

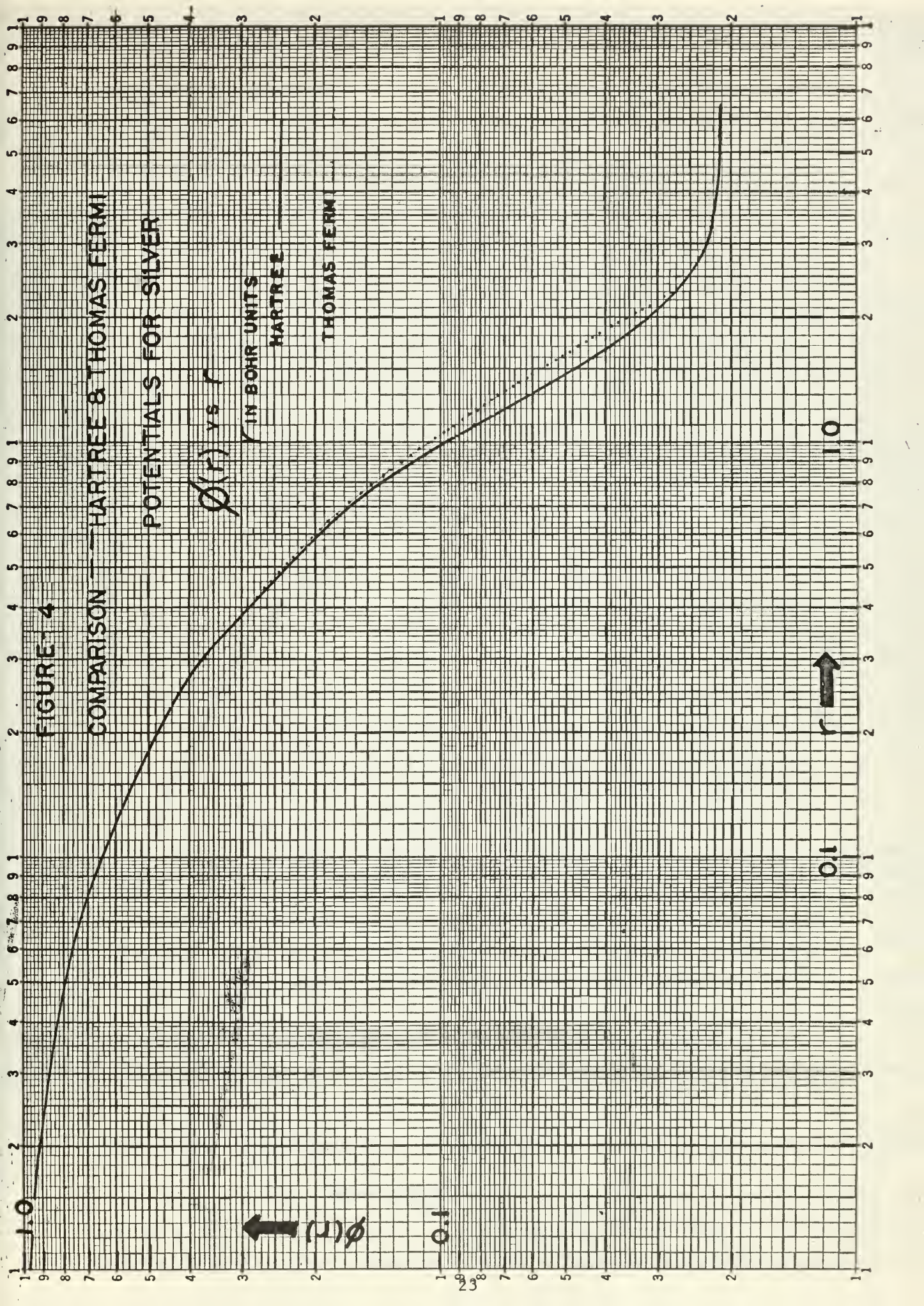
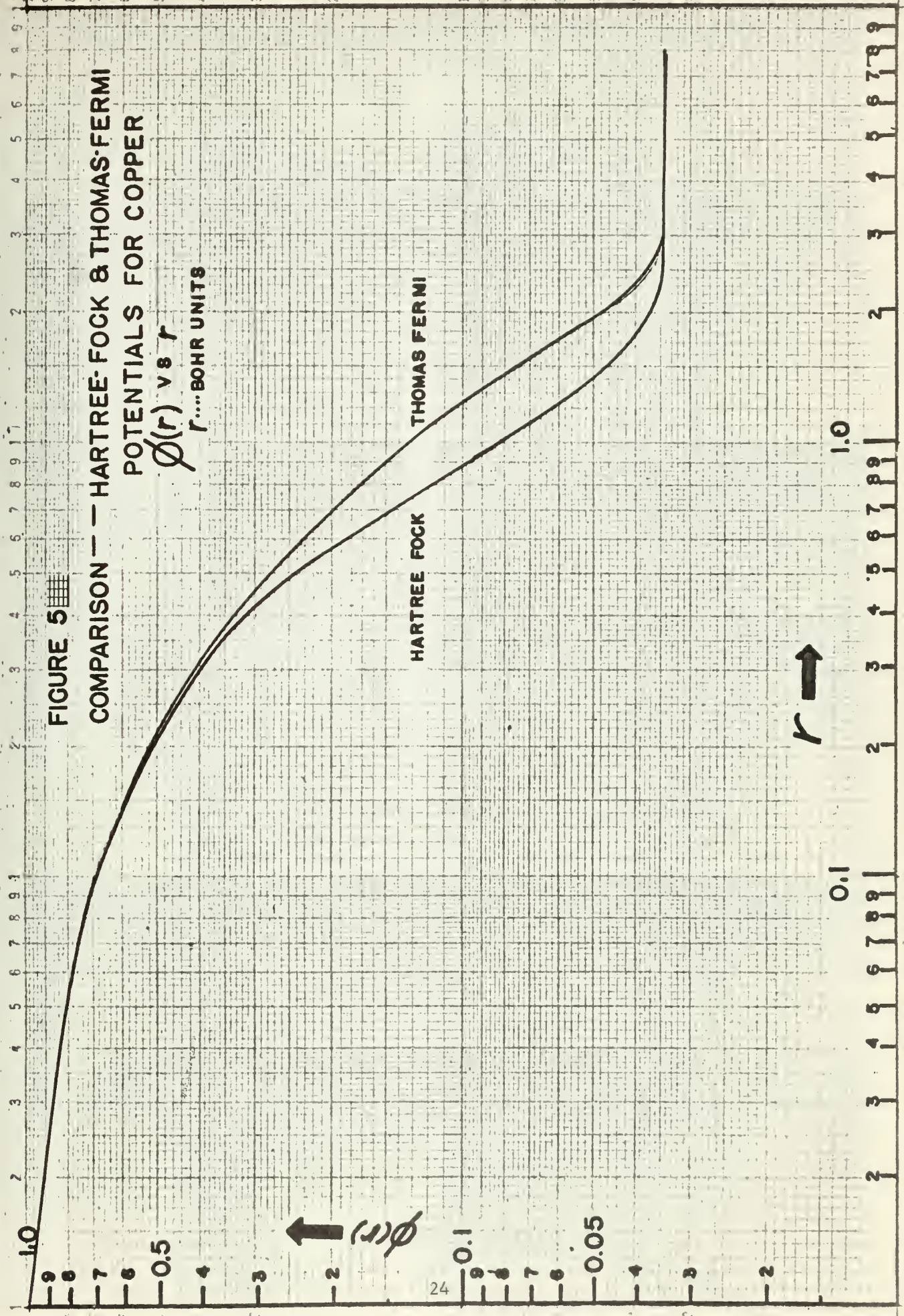
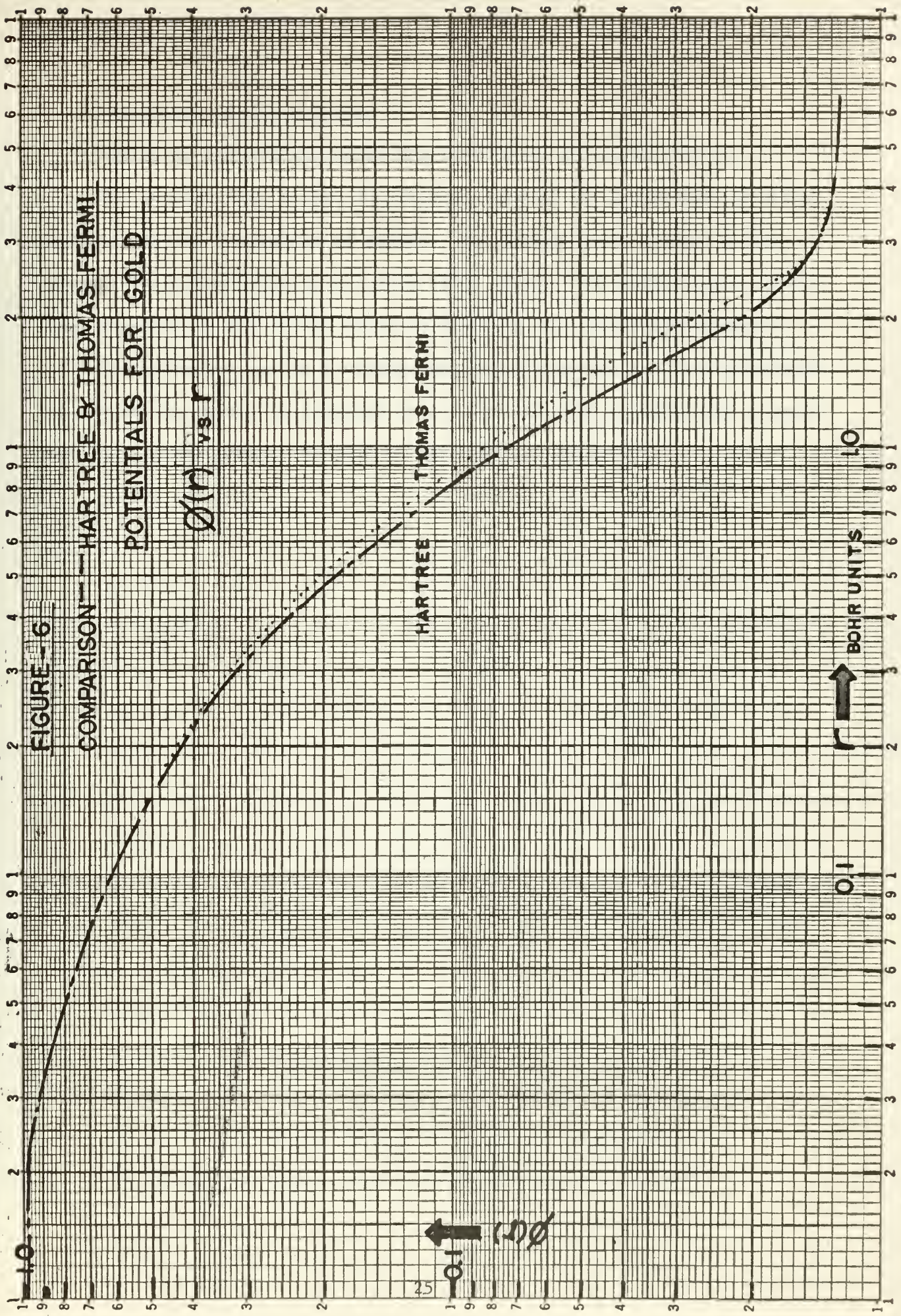


FIGURE 5

COMPARISON — — HARTREE-FOCK & THOMAS-FERMI
POTENTIALS FOR COPPER

$\phi(r)$ vs r
 r ...BOHR UNITS





Comparison of Calculations

Tables II and III summarize the results of the calculations.

The results were rather surprising, none of the potentials actually represented the ionization of energy. The Thomas-Fermi copper is the nearest to representing an accepted value (80%). The Hartree gold potential represented 52% of the accepted value of the ionization energy.

These results may be a strong indication that the ion core potential of a free ion should be replaced by a potential more suitable for a metal rather than corrections be made to the free ion potential.

TABLE II

Comparison of Calculations and Accepted Values for the Lowest Energy State and Atomic Radius of Copper, Silver, and Gold.

	Lowest Energy State (Rydbergs)	Atomic Radius (Bohr-Units)
<u>Copper</u>		
Hartree-Fock	.54	4.42
Thomas-Fermi	.87	3.13
<u>Silver</u>		
Hartree	.45	4.94
Thomas-Fermi	.44	4.34
<u>Gold</u>		
Hartree	.41	5.96
Thomas-Fermi	.41	4.60
Accepted values ^a		
Copper		2.65
Silver		3.01
Gold		3.01
Calculated by others ^b		
Copper		3.16

^aF. Seitz, The Modern Theory of Solids, op. cit. p. 6

^bF. Seitz, The Modern Theory of Solids, op. cit. p. 370

TABLE III

Comparison of Calculations and Accepted Values for the Ionization Energy and Cohesive Energy of Copper, Silver, and Gold.

	Ionization ^a Energy (Rydbergs)	Cohesive ^b Energy (K Cal/mole)
<u>Copper</u>		
Hartree-Fock	.33	24.0
Thomas-Fermi	.45	33.75
<u>Silver</u>		
Hartree	.30	18.6
Thomas-Fermi	.30	13.4
<u>Gold</u>		
Hartree	.35	--
Thomas-Fermi	.28	8.08
Accepted values		
Copper	.558 ^c	81.2 ^d
Silver	.547 ^c	69.0 ^d
Gold	.666 ^c	82.3 ^d
Calculated by others		
Copper		33 ^e
Gold		49 ^f

^aThe potential represents the calculated ionization energy.

^bThe value of the ionization energy represented by the potential was used in the calculation.

^cL. H. Ahrens and S. R. Taylor, Spectro Chemical Analysis (Addison-Wesley Publishing Co., Inc., Reading, Mass., 1961).

^dE. Wigner and F. Seitz, The Qualitative Analysis of the Cohesion in Metals, Advances in Research and Applications of Solid State Physics (Academic Press, New York 1955), Volume 1, p. 108.

^eF. Seitz, Modern Theory of Solids, op. cit., p. 370.

^fK. Kambe, Cohesive Energy of Noble Metals, Phys. Rev. 99, No. 2, 419-22 (15 June 1955).

DEVELOPMENT OF A NEW POTENTIAL FOR GOLD

The Model

An inspection of the results of the calculations for the noble metals and the results for sodium indicate two major differences: (1) The sodium potential actually represented the ionization energy, the others did not; and (2) the sodium results agree with experiment, the others did not. If a potential could be found which satisfied the ionization energy, the exchange energy and interaction energies would be taken into account. This statement would not be entirely correct except for a spherically symmetric model, unless the potential itself were a function of angle as well as position. If it were possible to construct a potential which does satisfy the ionization energy, which is spherically symmetric and would give results close to experiment, the simplicity of the original Wigner-Seitz method would be preserved.

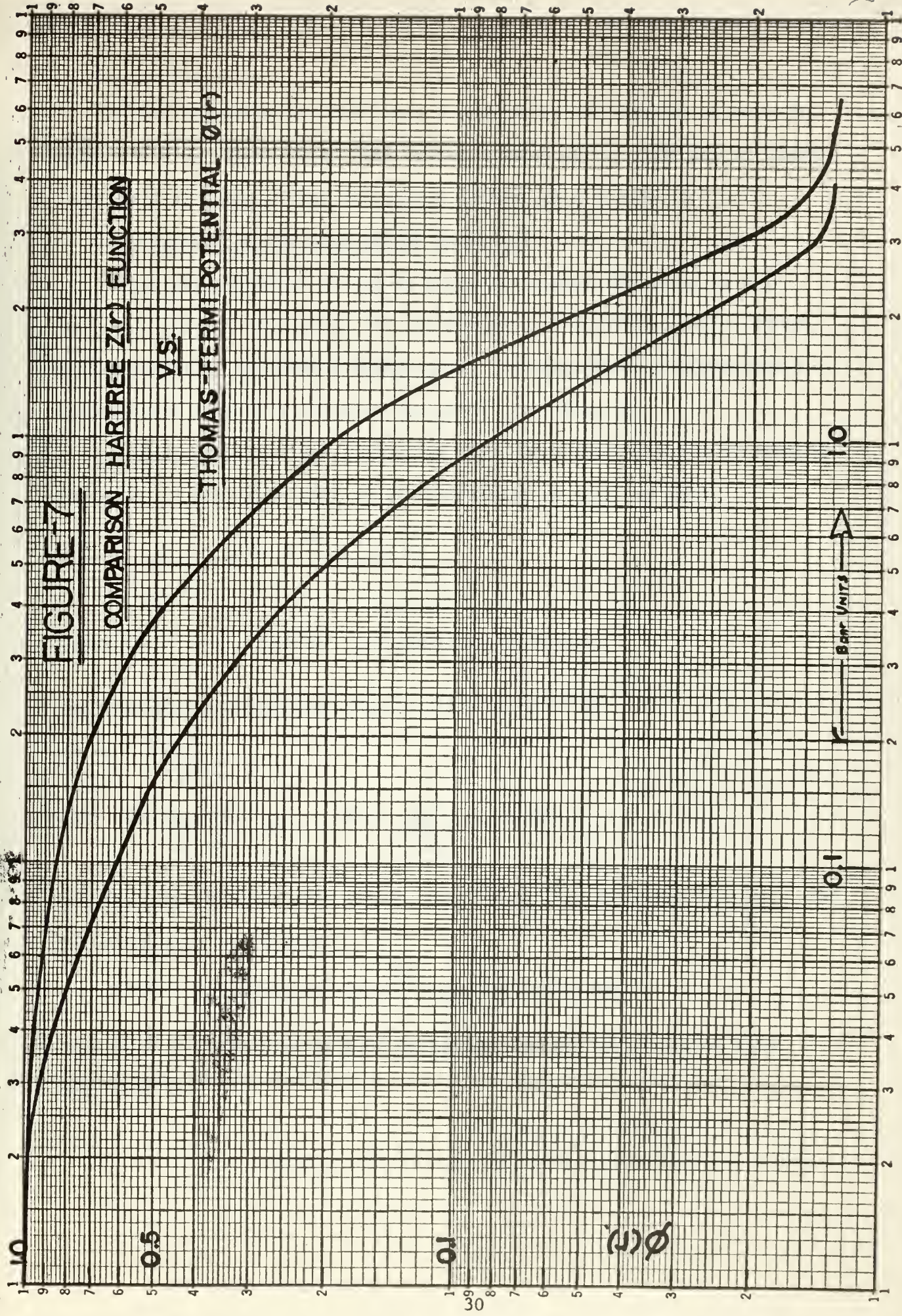
Starting the Problem

Fig. 7 shows the Hartree function $Z(r)$ and the Thomas-Fermi potential plotted on the same log-log plot. $Z(r)$ was substituted for $\phi(r)$ in the Wigner-Seitz calculation and was found to represent an ionization energy of approximately one Rydberg.

It was decided to try a variation of curves between the limits of the $Z(r)$ Hartree function and the Thomas-Fermi potential to determine which functions satisfied the ionization potential.

It is noted from Fig. 7 that the form of the $Z(r)$ function breaks at $r = 3.0$. The function then approaches $1/Z$ at approximately $r = 6.5$. This suggested considering the $\phi(r)$ as made up of three curves,

$$\begin{aligned} 0 &\leq r \leq 3.0 \\ 3.0 &\leq r \leq 6.5 \\ r &> 6.5 \end{aligned}$$



It was necessary to start some place, so it was decided to hold the point $r = 3.0$, $\phi(r) = 0.21$ (the values of $Z(r)$ at $r = 3.0$) and to insure continuity of slope of the two curves joining at $r = 3.0$.

Development of the Form of the Equations

Since the potential should be periodic between ion cores in the lattice a periodic potential was considered as a starting point. Since $\phi(r)$ is equal to one when r equals zero, a cosine function represents a satisfactory form of a periodic function. (See Fig. 8)

A decay parameter was introduced with the cosine function to develop the shape of the curve that is characteristic of $Z(r)$ and $\phi(r)$

$$\text{that is } \phi(r) = e^{-ST \cdot r^{SU}} \cos(SY \cdot r)$$

where ST , SY and SU are arbitrary functions.

The periodicity conditions require $\cos(SY \cdot r) = 0$

$$\text{where } r = \frac{A_0}{4}$$

$$\text{Thus } SY \cdot \frac{A_0}{4} = \frac{\pi}{2} \quad \text{OR} \quad SY = \frac{2\pi}{A_0} = 1.825$$

In order that $\phi(r)$ be some finite value other than zero when $r = \frac{A_0}{4}$ the following form was chosen:

$$\phi(r) = (1-SX) \exp(-ST \cdot r^{SU}) \cos(SY \cdot r) + SX$$

Thus $\phi(r)$ is a function of four parameters and has the required form.

(See Fig. 9)

In the range $3.0 \leq r \leq 6.5$, $\phi(r)$ was assumed to vary as $1/r$ with the equation

$$\phi(r) = .021 \frac{(3+SB)}{(r+SB)} \quad (\text{See Fig. 10})$$

using the condition $r = 6.5$, $\phi(r) = \frac{1}{Z}$

$$\longrightarrow \frac{1}{Z} = .021 \frac{(3+SB)}{(6.5+SB)}$$

solving the equation for SB yields $SB = 2.0$

therefore

$$\phi(r) = \frac{.110}{r+2.0} \quad 3.0 \leq r \leq 6.5$$

Satisfying the Boundary Conditions

The first condition is: $\phi(r) = .021$ $r = 3.0$

$$\longrightarrow .021 = (1-SX) \exp(-ST \cdot 3^{\text{SU}}) \cos(3 SY) + SX$$

solving for $\exp(ST \cdot 3^{\text{SU}})$

$$\exp(ST \cdot 3^{\text{SU}}) = \frac{(1-SX) \cos(SY \cdot 3)}{(.021 - SX)}$$

taking the natural logarithm of both sides

$$ST \cdot 3^{\text{SU}} = \text{LN} \left(\frac{(1-SX) \cos(3 SY)}{(.021 - SX)} \right)$$

taking the natural logarithm of both sides and solving for SU

$$SU = \frac{1}{\text{LN } 3.0} \left\{ \text{LN} \left[\text{LN} \left(\frac{(1-SX) \cos(3 SY)}{(.021 - SX)} \right) \right] - \text{LN } ST \right\}$$

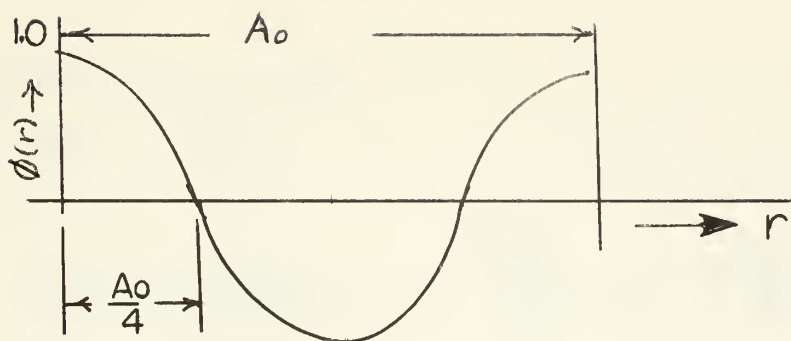


Fig. 8. First Approximation to a Periodic Potential Between Ion Cores.
 A_0 equals the edge length of the fundamental cube of a cubic lattice.

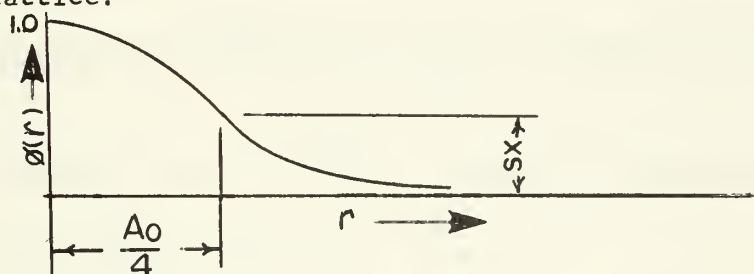


Fig. 9 Graphical Portrayal of the Equation $\phi(r) = (1 - SX) \exp(-STr^{1/2}) \cos SYr + SX$
 SY equals $A_0/4$, SX is the value of $\phi(r)$ when $SY \cdot r$ equals $\pi/2$
 This equation applies in the region $0 \leq r \leq 3.0$ Bohr Units.

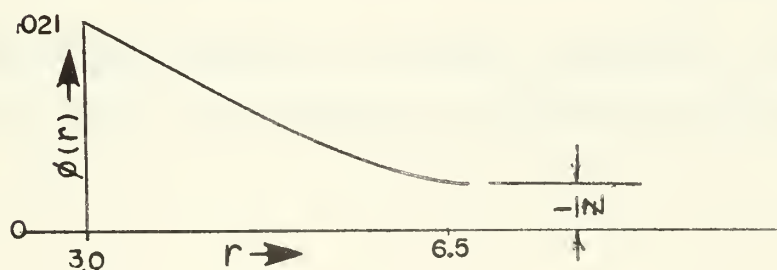


Fig. 10. Graphical Portrayal of the Equation $\phi(r) = \frac{.110}{(2.0+r)}$
 This equation applies in the range $3.0 \leq r \leq 6.5$ Bohr Units.
 Z is the atomic number.

To satisfy continuity of slope

$$\phi(r) = \frac{.110}{r+2}$$

$$\phi'(r) = -\frac{.110}{(r+2)^2} = -\frac{\phi(r)}{r+2} = -\frac{.021}{5}$$

from the first equation

$$\phi'(r) = (1-SX) \cdot \exp(-ST \cdot r^{SU}) \left[-SY \cdot \sin(SY \cdot r) - \cos(SY \cdot r) \cdot ST \cdot SU \cdot r^{SU-1} \right]$$

This simplifies to

$$\phi'(r) = (1-SX) \exp(-ST \cdot r^{SU}) \cos(SY \cdot r) \left[-SY \cdot \tan(SY \cdot r) - ST \cdot SU \cdot \frac{r^{SU}}{r} \right]$$

$$\text{since } (1-SX) \exp(-ST \cdot r^{SU}) \cdot \cos(SY \cdot r) = \phi(r) - SX$$

introducing the values of $\phi(r)$ at $r = 3.0$

$$-\frac{.021}{5} = -(.021 - SX) \left(SY \cdot \tan(3 \cdot SY) - SU \cdot ST \cdot \frac{3^{SU}}{3} \right)$$

$$\text{Let } ST \cdot 3^{SU} = SZ$$

solving for SU

$$SU = \left(\frac{.021}{5(.021 - SX)} - SY \cdot \tan(3 \cdot SY) \right) \frac{3}{SZ}$$

This value of SU satisfies both boundary conditions. To differentiate between the values of the parameters satisfying one or two boundary conditions

Let SU satisfy one boundary condition and be described by equation

$$SU = \frac{1}{LN \ 3.0} \left\{ LN \ LN \left(\frac{(1-SX) \cdot \cos(3 \cdot SY)}{.021-SX} \right) - LN \ ST \right\}$$

ST is a parameter in the equation satisfying one boundary condition.

$$SUI = \frac{3}{SZ} \left(\frac{.021}{5(.021-SX)} - SY \cdot \tan(3 \cdot SY) \right)$$

$$SZ = SA \cdot 3^{SUI}$$

SZ is a parameter used in the equation satisfying two boundary conditions.

The reason for the above step is not obvious but will become clear in the next section.

The relationship between SA , $LN \ SX$, and SY is portrayed in Fig. 11. Each point meets the two boundary conditions (1) holding the point $\emptyset(r) = .021$ at $r = 3.0$, (2) continuity of slope at $r = 3.0$.

If one boundary condition is held constant $\emptyset(r) = .021$ at $r = 3.0$ (Fig. 12) and a fixed value of SX and SY are substituted in the cellular calculation for $E = .666$ Rydbergs, then ST is varied until a value of ST brackets the ionization energy. That is, in Fig. 13 the value of $R(r)$ changes from minus to plus.

In this manner the SY curves are developed by varying SX .

When the two curves are superimposed the intersection meets all the boundary conditions (Fig. 14). This procedure proved necessary as the slope of SX/SA was very flat and made location of the point of intersection difficult when all the conditions were wrapped into one equation. In this method there are two curves intersecting at right angles and it is easier

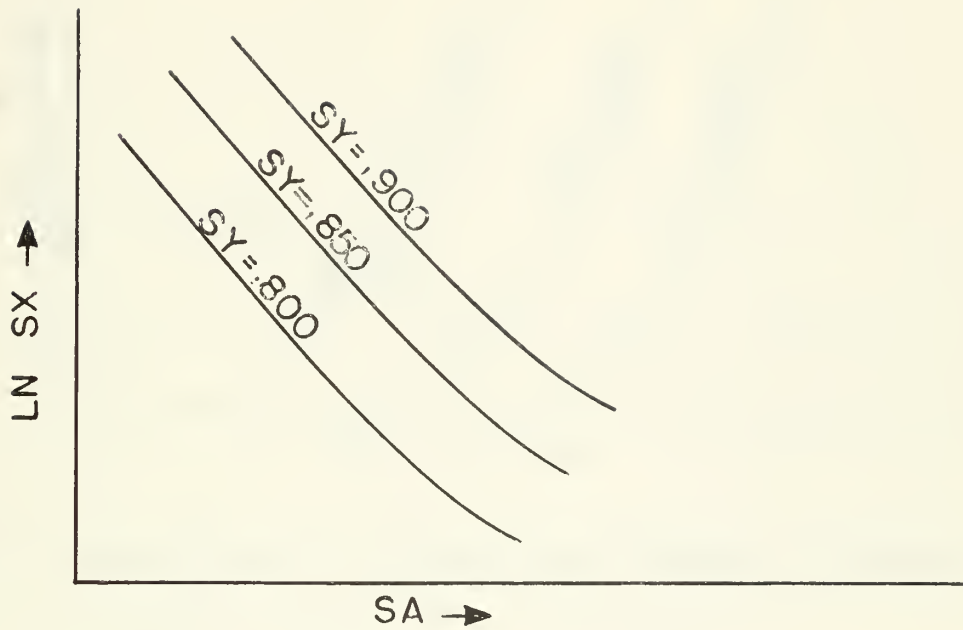


Fig. 11. The First Step in the Variational Procedure. A Semi-Log Plot of Curves of Constant SY vs. SX and SA.

Points on the SY curve satisfy the boundary conditions

$\emptyset(r) = .021$ at $r = 3.0$ and continuity of slope at $r = 3.0$.

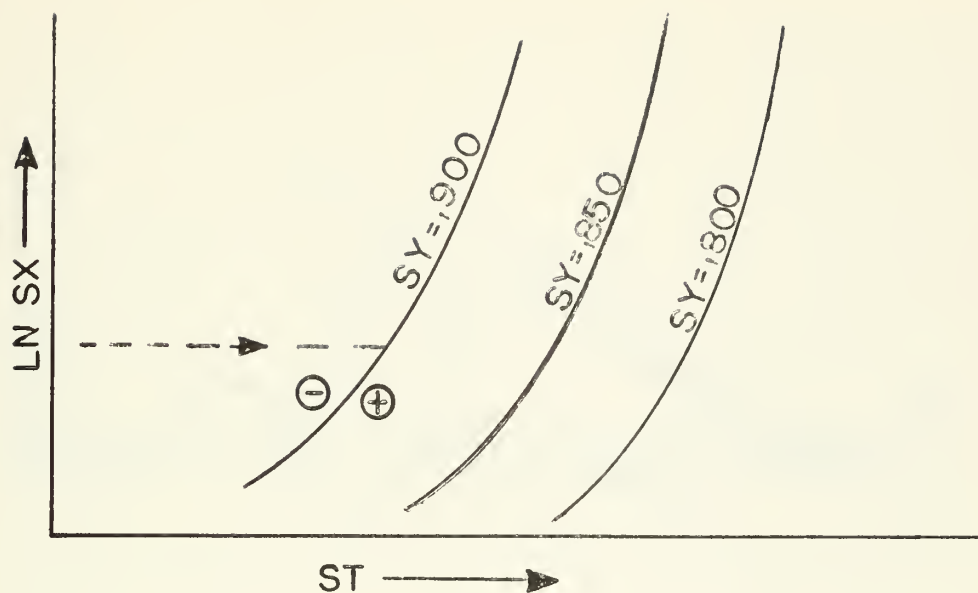


Fig. 12. The Second Step in the Variational Procedure. A Semi-Log Plot of Curves of Constant SY vs. $\ln SX$ and ST .

Points on the SY curves satisfy the boundary conditions: the ionization = .666 Rydbergs and $\phi(r) = 0.21$ at $r = 3.0$.

Initially SX and SY are held constant and ST is varied. The triad SY , ST and SX determine $\phi(r)$. The radial wave function $R(r)$ is determined by $\phi(r)$. When $R(r)$ changes sign at $r = 8.2$ Bohr units the ionization energy is satisfied. Keeping SY constant and using incremental values of SX , the procedure is repeated, giving the curves $SY = \text{constant}$.

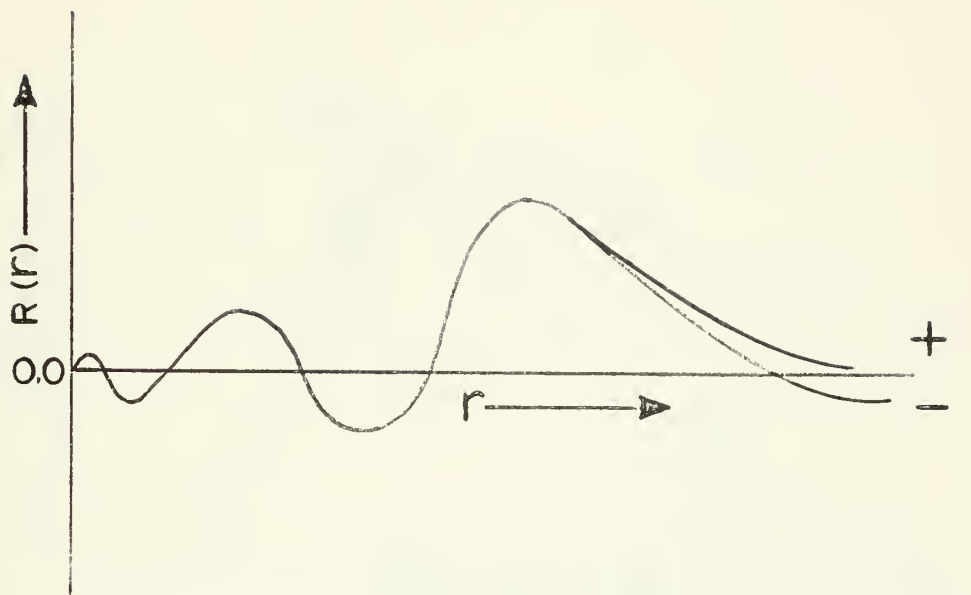


Fig. 13. Determination of the Ionization Energy.

The wave function $R(r)$ which satisfies the ionization energy lies between the limits of the curves marked + and -.

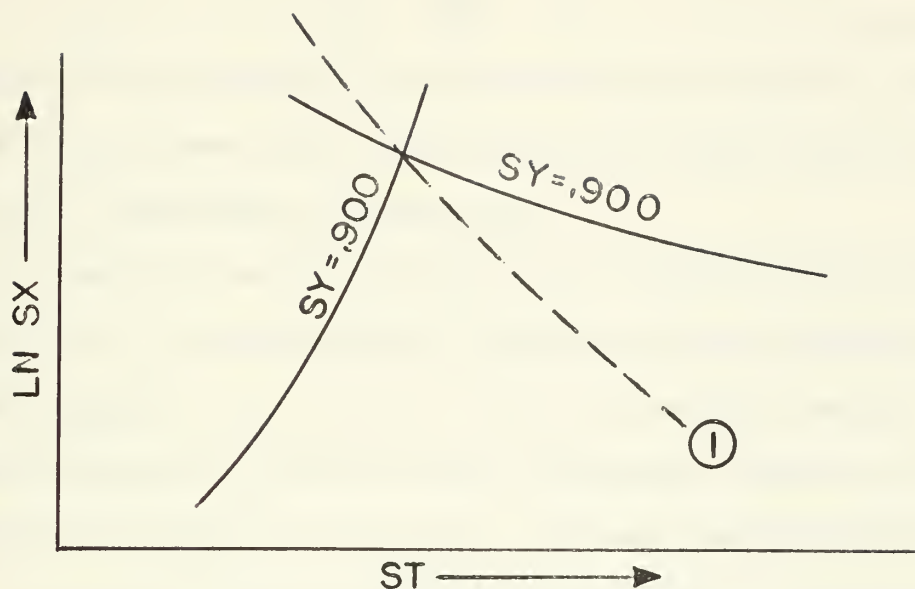


Fig. 14. Step Three of the Variation Procedure.

This plot is a superposition of Figs. 11 and 12. The point of intersection of curves of constant SY satisfy the boundary conditions $\phi(r) = 0.21$ at $r = 3.0$, continuity of slope at $r = 3.0$ and the ionization energy = .666 Rydbergs. The curve marked ① represents the locus of points satisfying the boundary conditions for various values of SY .

to select the intersection.

The results of the variation indicated that the boundary conditions were met along the curve marked (1) in Fig. 14. This was surprising. An additional criterion was then invoked that was to pick the curve which gave either the lowest energy state or values of atomic radius and cohesive energy that corresponded to known values.

The results of the first variation are tabulated in Table IV. (See also Fig. 15.) A second series of variations was made perturbing the boundary condition $r = 3.0$, $\phi(r) = .021$. This boundary condition was originally selected as starting point by observing a break in the shape in the Hartree $Z(r)$ curve at this point. The entire procedure depicted in Figs. 11 through 15 was repeated for new dyad $\phi(r)$, r , representing a new boundary condition. The second variation was terminated when the accepted value of the atomic radius was obtained. The results of the second variation are tabulated in Table IV. It is noted that the cohesive energy from the derived potential, 81.6 Rydbergs, compares very well with the accepted value 83.5 Rydbergs.

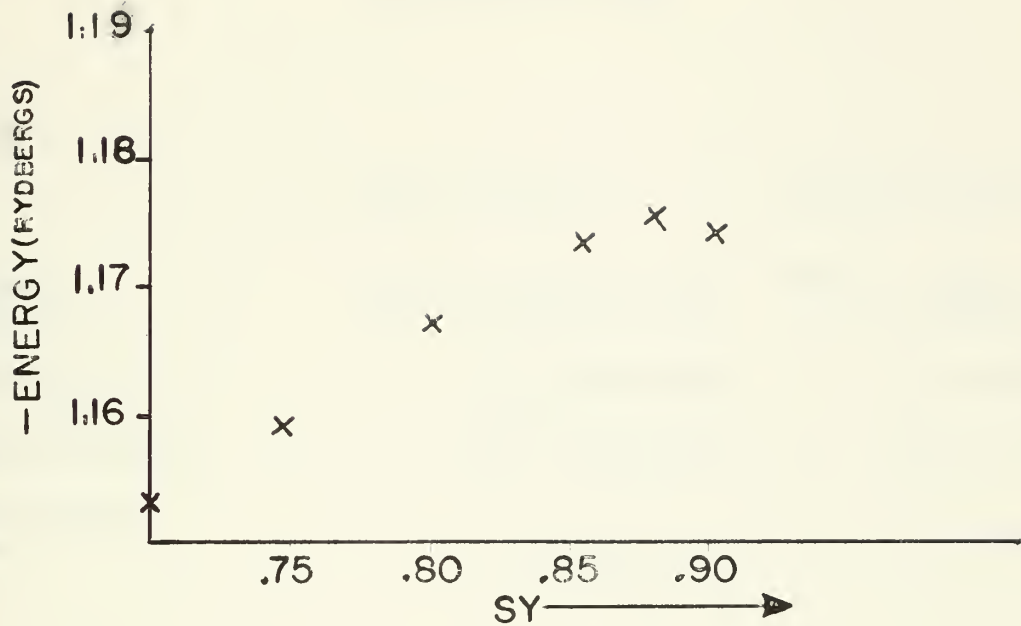


Fig. 15. Plot of Values of the Lowest Energy State vs. SY Satisfying the Boundary Condition, the Ionization Energy = .666 Rydbergs. The values of SY giving the lowest value of the energy state represents the triad of parameters from curve (1) in Fig. 14. This triad determines $\phi(r)$.

TABLE IV
RESULTS OF THE FIRST AND SECOND
VARIATIONS FOR GOLD

	First Variation	Second Variation
Boundary Condition	$\phi(r) = .021$ $r = 3.0$ Bohr units	$\phi(r) = .020$ $r = 2.99$ Bohr units
Atomic Radius ^a	3.13 Bohr units	3.01 Bohr units
Cohesive Energy ^b	80.6 K Cal/Mole	81.6 K Cal/Mole
Lowest Energy State	1.172 Rydbergs	1.194 Rydbergs

Note: ^aAccepted Value of $r_o = 3.01$ Bohr units.

^bAccepted Value of Cohesive Energy = 83.5 K Cal/Mole

CONCLUSIONS AND SUMMARY OF RESULTS

It proved possible to construct a potential for gold which can be expressed in a closed form and when used in the cellular method can furnish very close agreement with accepted values of the atomic radius and the cohesive energy. This potential is a central field potential and represents a spherically symmetric model. The potential $V(r)$ is expressed in terms of a function, $\phi(r)$, which is the normalized contribution to the effective potential.

$$\phi(r) = .9174 \exp(-1.429 r^{.524676}) \cos(.875r) + .0826$$

$$0 \leq r \leq 2.99 \quad \text{Bohr units}$$

$$\phi(r) = \frac{.121}{3.062 + r}$$

$$2.99 \leq r \leq 6.5 \quad \text{Bohr units}$$

$$\phi(r) = \frac{1}{79}$$

$$r \geq 6.5 \quad \text{Bohr units}$$

Fig. 16 graphically portrays the complete Wigner-Seitz Cellular Computation for gold using the potential as described above.

It is very difficult to find any work on gold with which to compare our results. Kambe²² made a calculation of the cohesive energy of gold

²²K. Kambe, Phys. Rev. 99, No. 2, 419-22 (July 15, 1955)

FIGURE 16

GOLD

LOWEST ENERGY STATE

① INCLUDES FERMI ENERGY

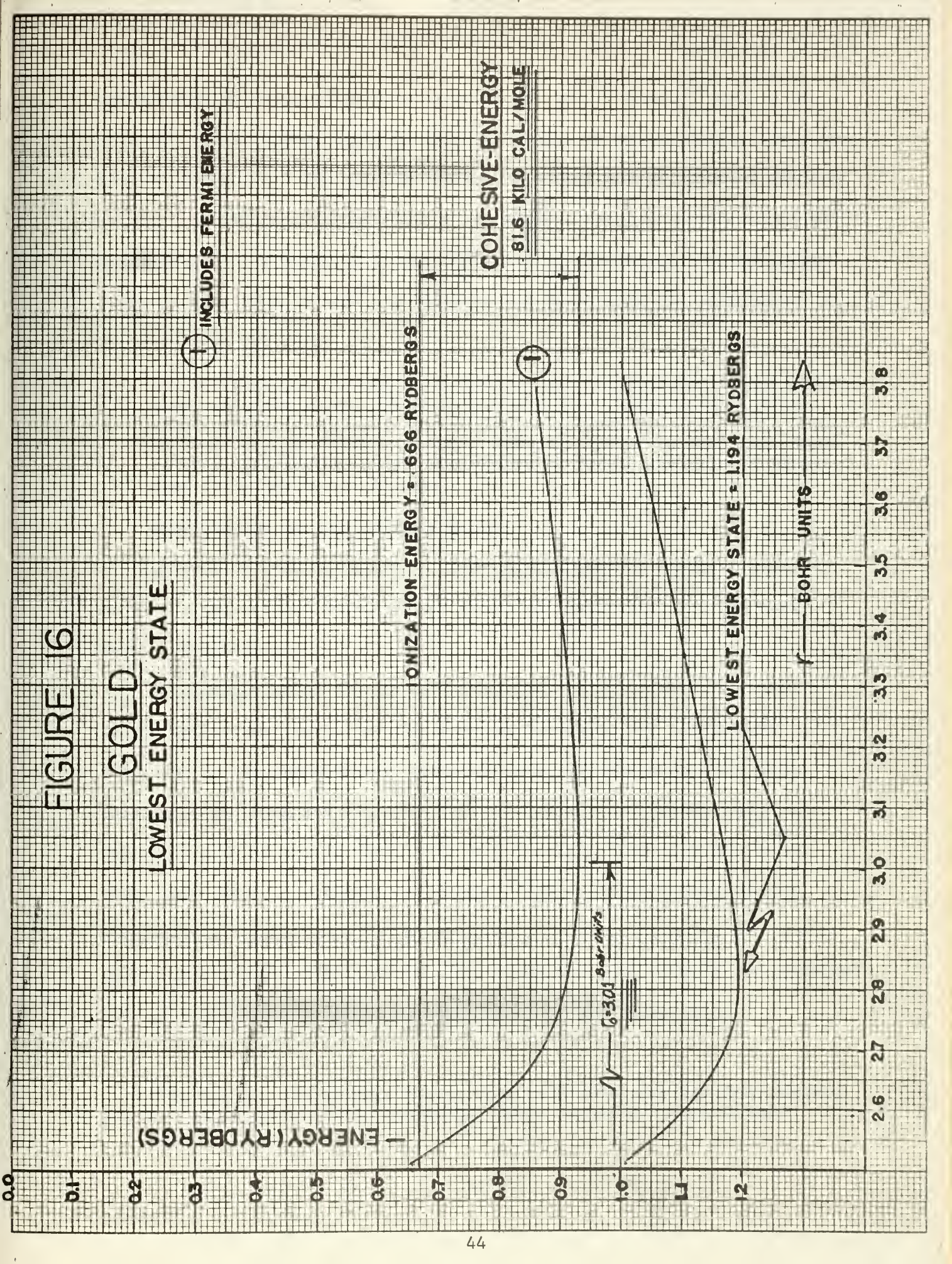
IONIZATION ENERGY = 666 RYDBERGS

COHESIVE-ENERGY

81.6 KILO CAL/MOLE

LOWEST ENERGY STATE = 1194 RYDBERGS

r — BOHR UNITS



and obtained a value of 49 kilo calories per mole. Segall²³ made a calculation of the energy bands in gold at lattice symmetry points using the Hartree Potential. His results indicate a lowest energy state of approximately 1.25 Rydbergs in the (0,0,0) and $\frac{2\pi}{a}$ (1/2,1/2,1/2) direction, and approximately 1.3 Rydbergs in the $\frac{2\pi}{a}$ (1,0,0) direction. The following quote is made from Segall²³ to indicate his opinion on the uncertainty of the potential for gold.

The difficulties already discussed for Ag, in obtaining a good potential, are more severe for Au because it is a considerably heavier atom. Also, at present, only Hartree functions are available. Thus we would expect considerably more uncertainty in the potential which we have constructed in the same manner as for Cu and Ag, and consequently in the final results.

Contribution to the Cohesive Energy

There is a marked difference between the cohesive energy calculated using the Hartree and Thomas-Fermi Potential (Table III) and the newly developed potential.

An examination of the wave function $R(r)$ of the state corresponding to the ionization energy for the free ion potential for the Hartree (Fig. 70) or the Thomas-Fermi Potential (Fig. 63) indicates a 6S wave function. If these are compared with the radial wave function $R(r)$ of the calculated potential (Fig. 17), or $\psi(r)$ (Fig. 18) or $\tilde{\psi}(r)$, $\tilde{\psi}^*(r)$ (Fig. 19), there is a marked difference. The first difference is the new potential indicates a 7S instead of a 6S state. Secondly, the inner shells appear more tightly bound. One interpretation based on the examination of the functions discussed above would be that there is a

²³B. Segall, Theoretical Energy Band Structures for the Noble Metals (General Electric Research Laboratory, 1961) Report Nr. 61 R1(2785G)

FIGURE 17
GOLD

RADIAL WAVE FUNCTION $R(r)$ vs.
RADIAL DISTANCE r
ENERGY STATE $E = .666$ RYDBERGS
IONIZATION ENERGY

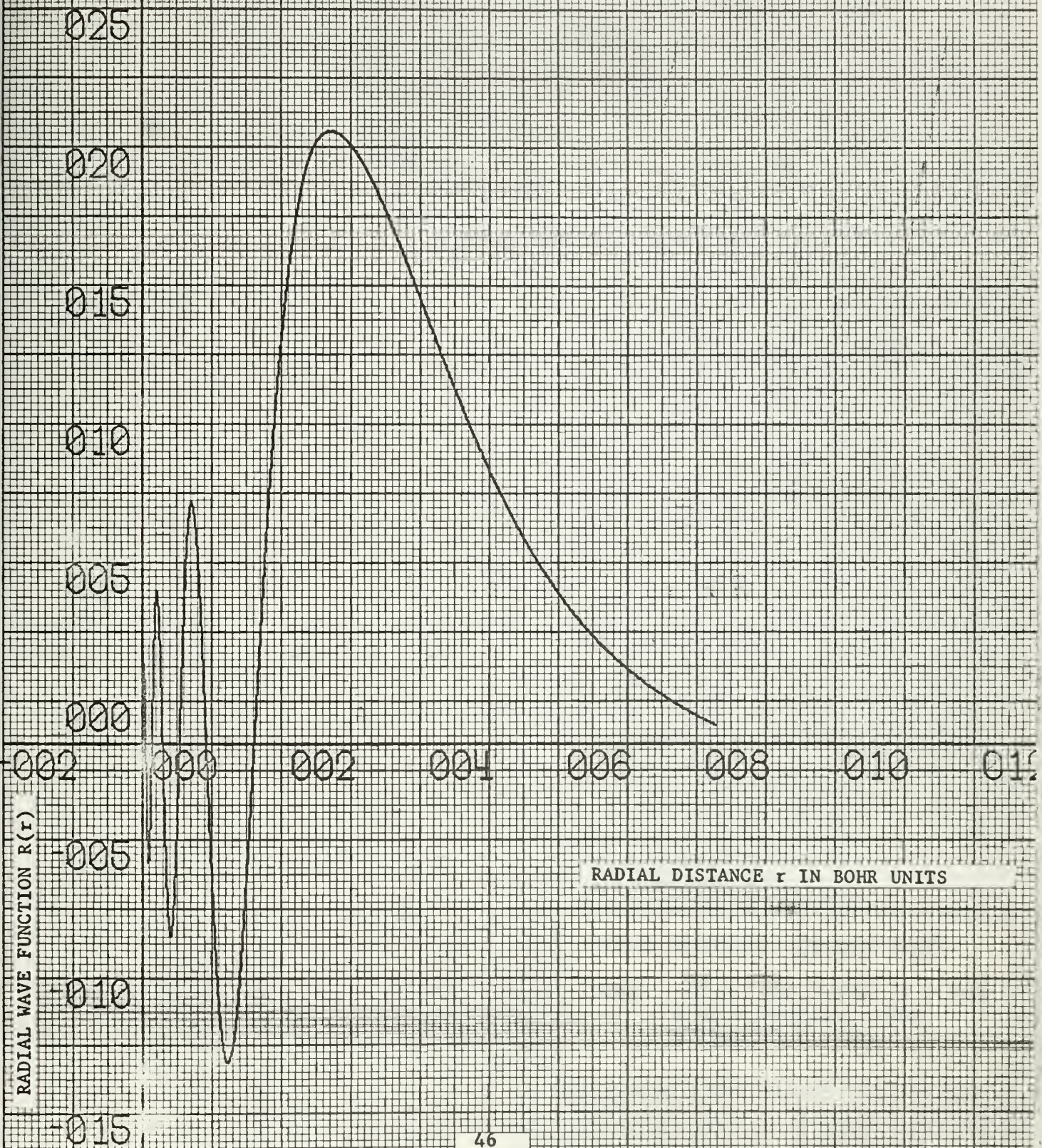


FIGURE 18

GOLD

RADIAL WAVE FUNCTION $\psi(r)$ vs.

RADIAL DISTANCE r

ENERGY STATE $E = .666$ RYDBERGS

IONIZATION ENERGY

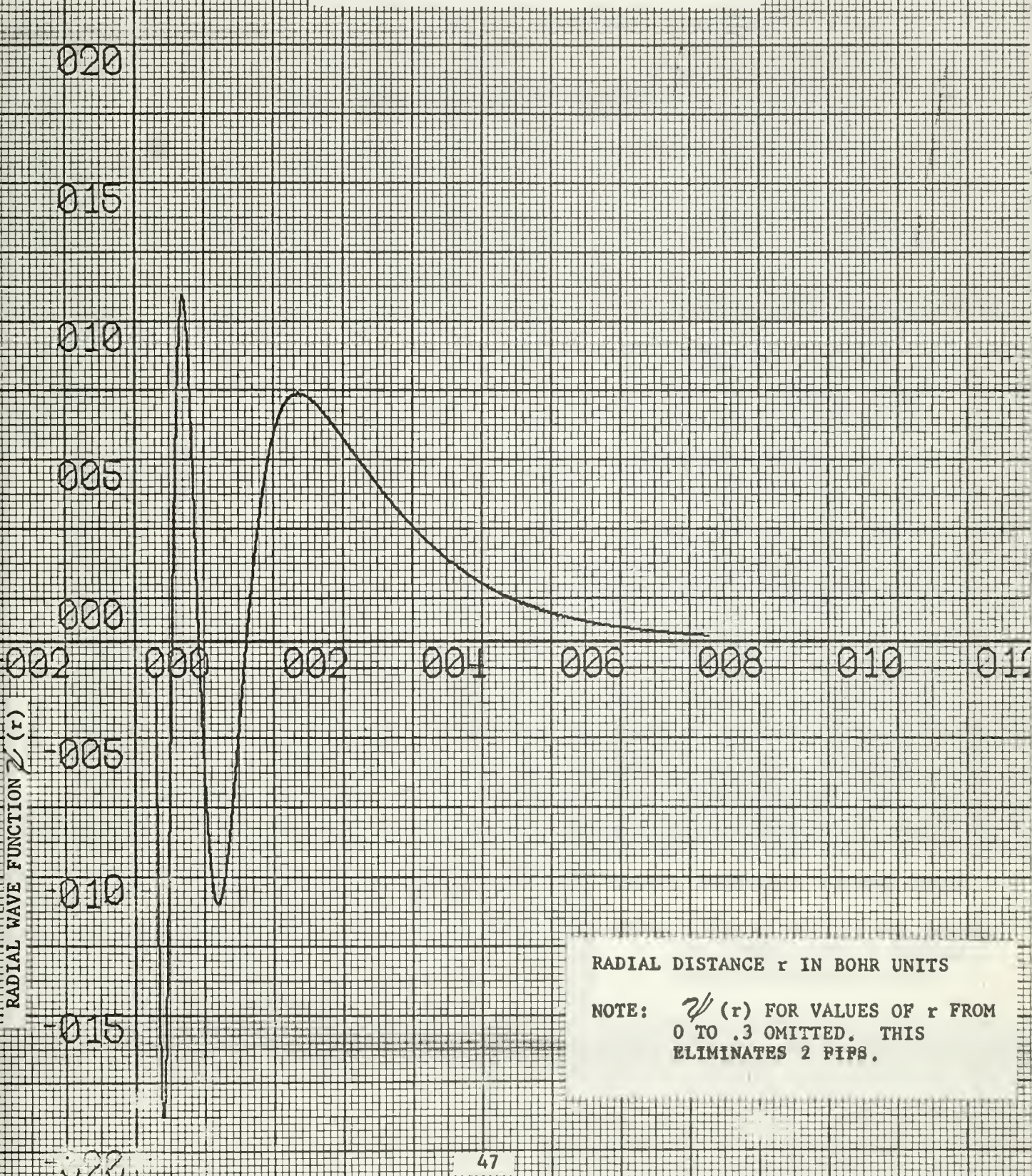


FIGURE 19

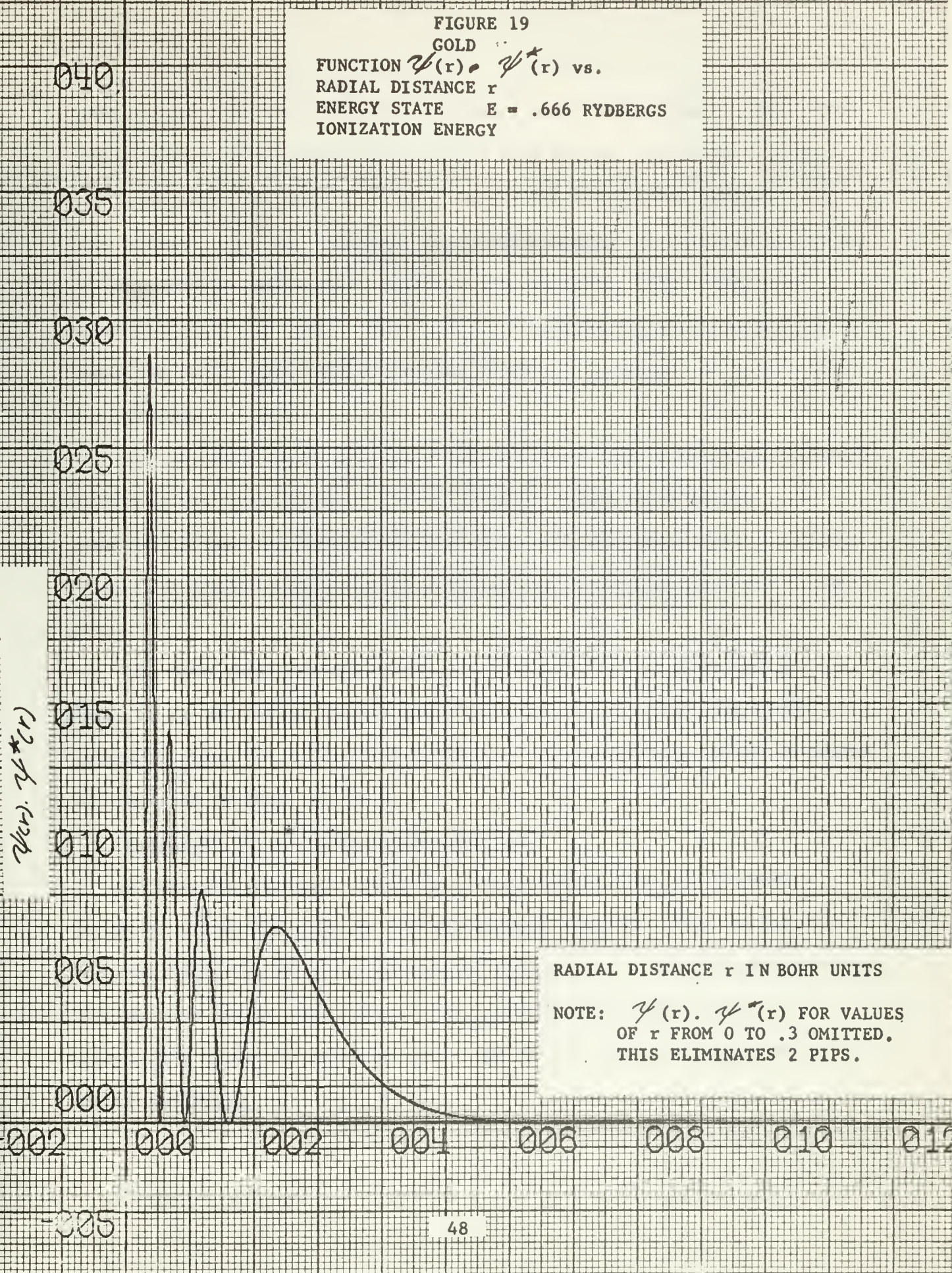
GOLD

FUNCTION $\psi(r)$, $\psi^*(r)$ vs.

RADIAL DISTANCE r

ENERGY STATE $E = .666$ RYDBERGS

IONIZATION ENERGY



redistribution of the electrons in a metal when compared with a free ion. The 6s appears to be more tightly bound than the 5f. There is a strong indication that there is a material overlap of these outer orbitals. It thus appears that the difference in cohesive energy is accounted for by a strong exchange interaction between the 5f orbitals. The difference between the two calculated values, 8.08 K Cal/Mole for the Thomas-Fermi potential and 81.6 K Cal/Mole for the developed potential, is substantial and striking.

The validity of the physical interpretation must of course be tempered by the assumptions that went into the model for the calculations. It appears that the calculation in this paper indicates the limit of a Wigner-Seitz cellular calculation using a spherically symmetric model for a heavy metal.

The wave functions for the lowest energy state are indicated in Figs. 20 to 22. It is noted that $\psi(r)$ is practically flat over a considerable range of r . The wave functions for intermediate values of energy are depicted in Figs. 23 to 26.

Extension of the Variational Technique

It appears possible, using the present calculations to develop a potential which when used in the Schrodinger equation would satisfy the boundary condition on the Wigner-Seitz polyhedron. It may be surmised that the cohesive energy calculated in this manner would differ from the spherically symmetric model by only 1.5% (83.5 K Cal/Mole, compared to 81.6 K Cal/Mole).

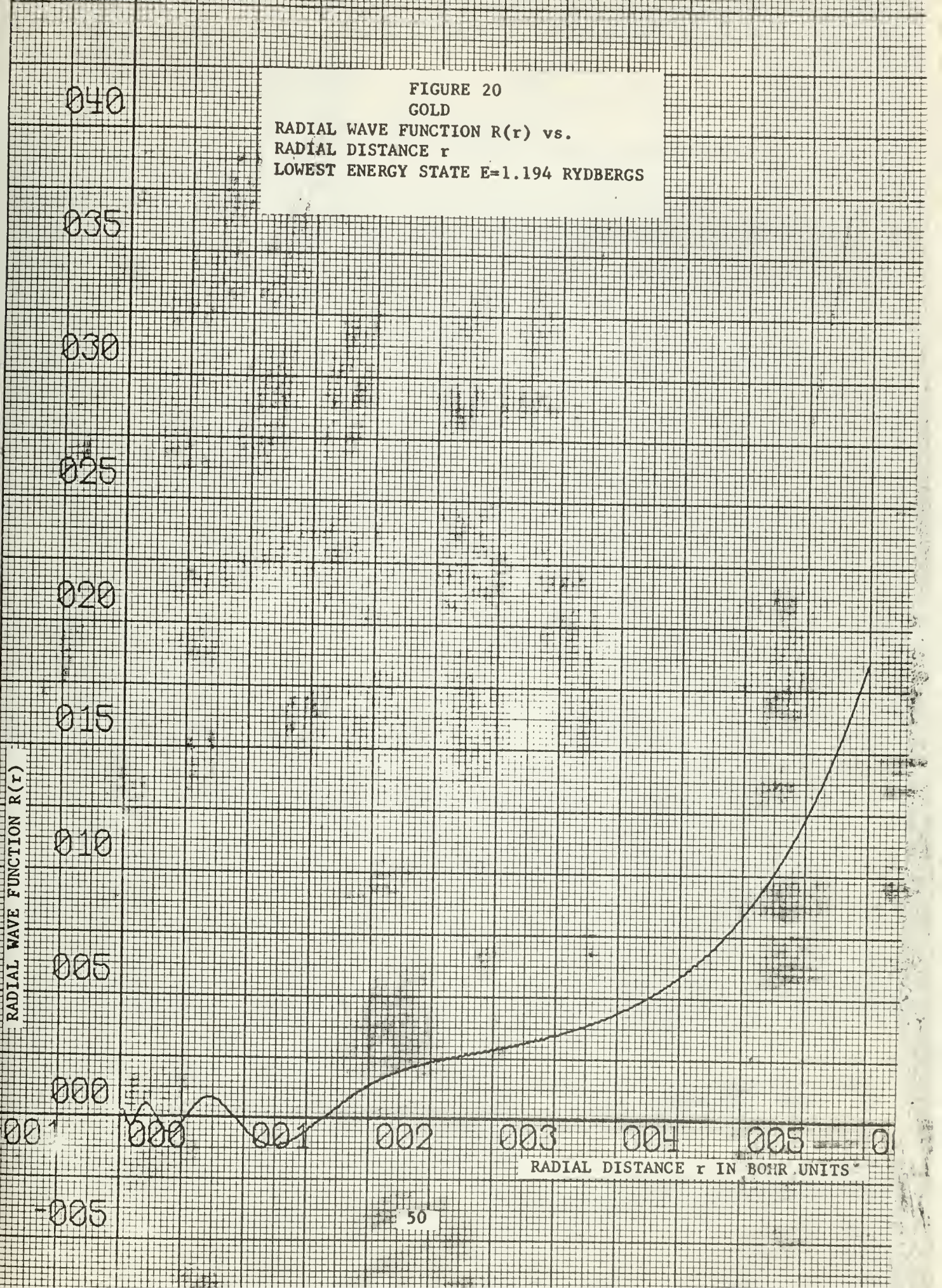
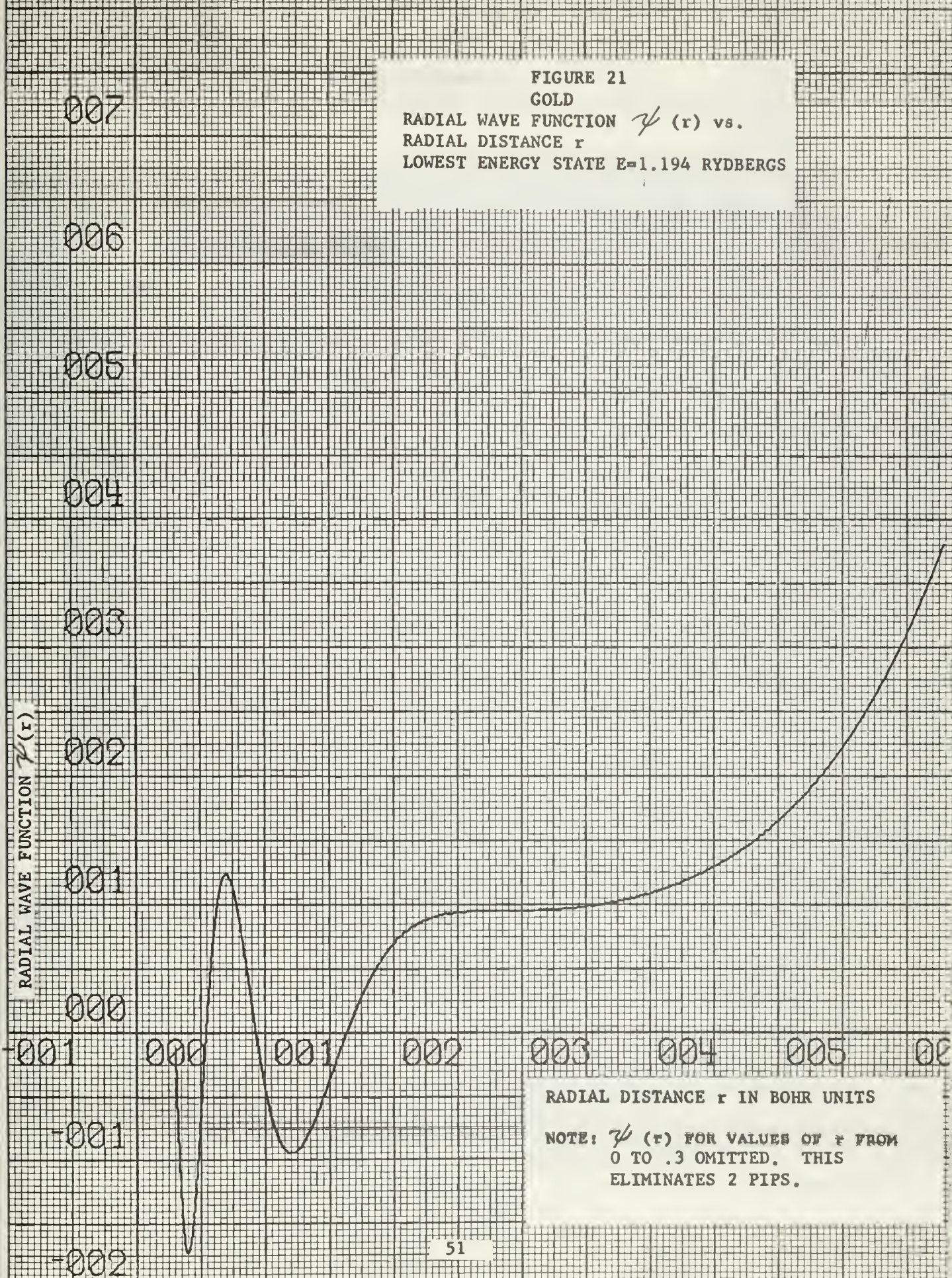


FIGURE 21
GOLD
RADIAL WAVE FUNCTION $\psi(r)$ vs.
RADIAL DISTANCE r
LOWEST ENERGY STATE $E=1.194$ RYDBERGS

RADIAL WAVE FUNCTION $\psi(r)$

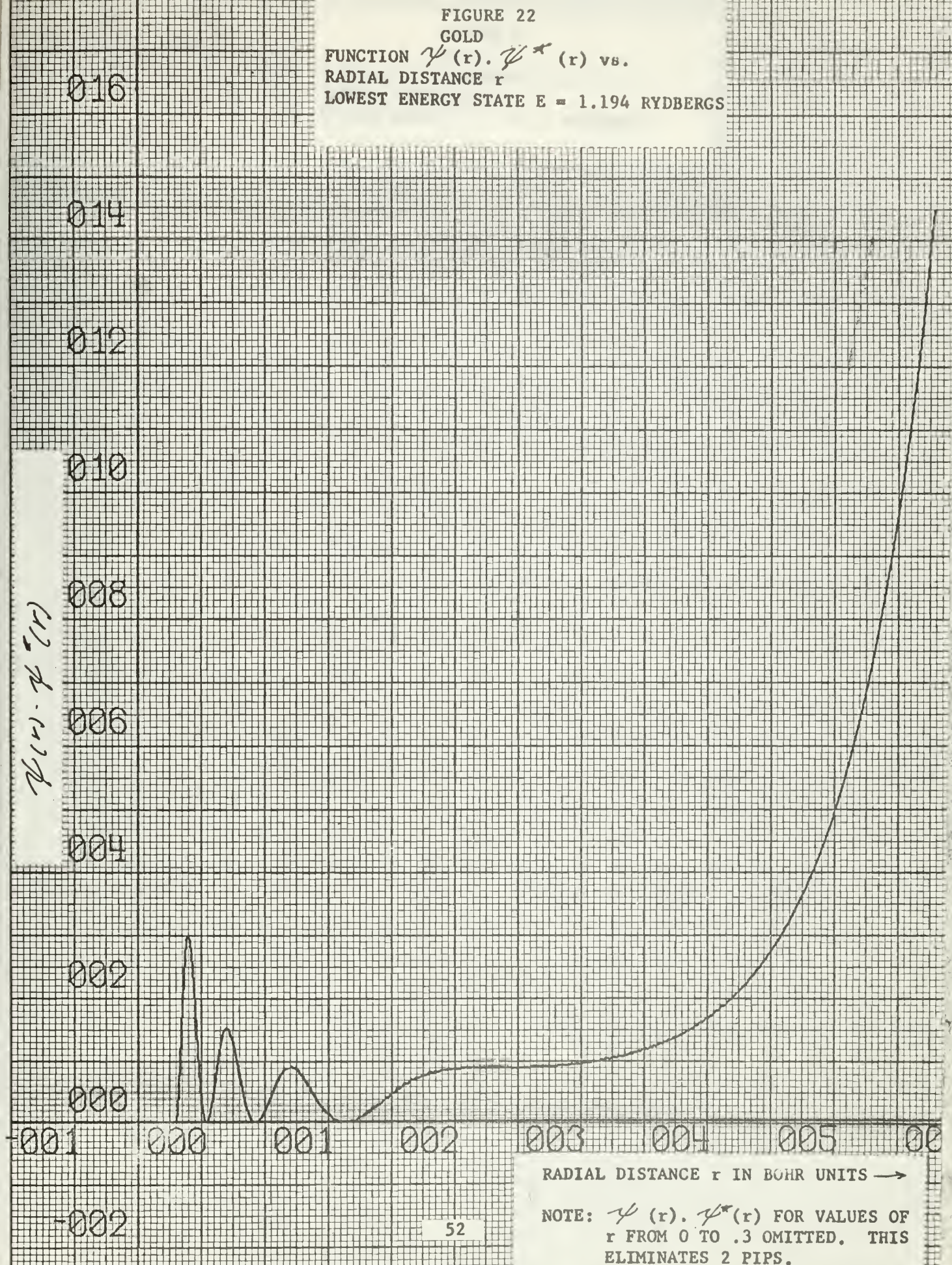


RADIAL DISTANCE r IN BOHR UNITS

NOTE: $\psi(r)$ FOR VALUES OF r FROM
0 TO .3 OMITTED. THIS
ELIMINATES 2 PIPS.

FIGURE 22

GOLD

FUNCTION $\psi(r) \cdot \psi^*(r)$ vs.RADIAL DISTANCE r LOWEST ENERGY STATE $E = 1.194$ RYDBERGSRADIAL DISTANCE r IN BOHR UNITS $\rightarrow$

NOTE: $\psi(r) \cdot \psi^*(r)$ FOR VALUES OF r FROM 0 TO .3 OMITTED. THIS ELIMINATES 2 PIPS.

FIGURE 23

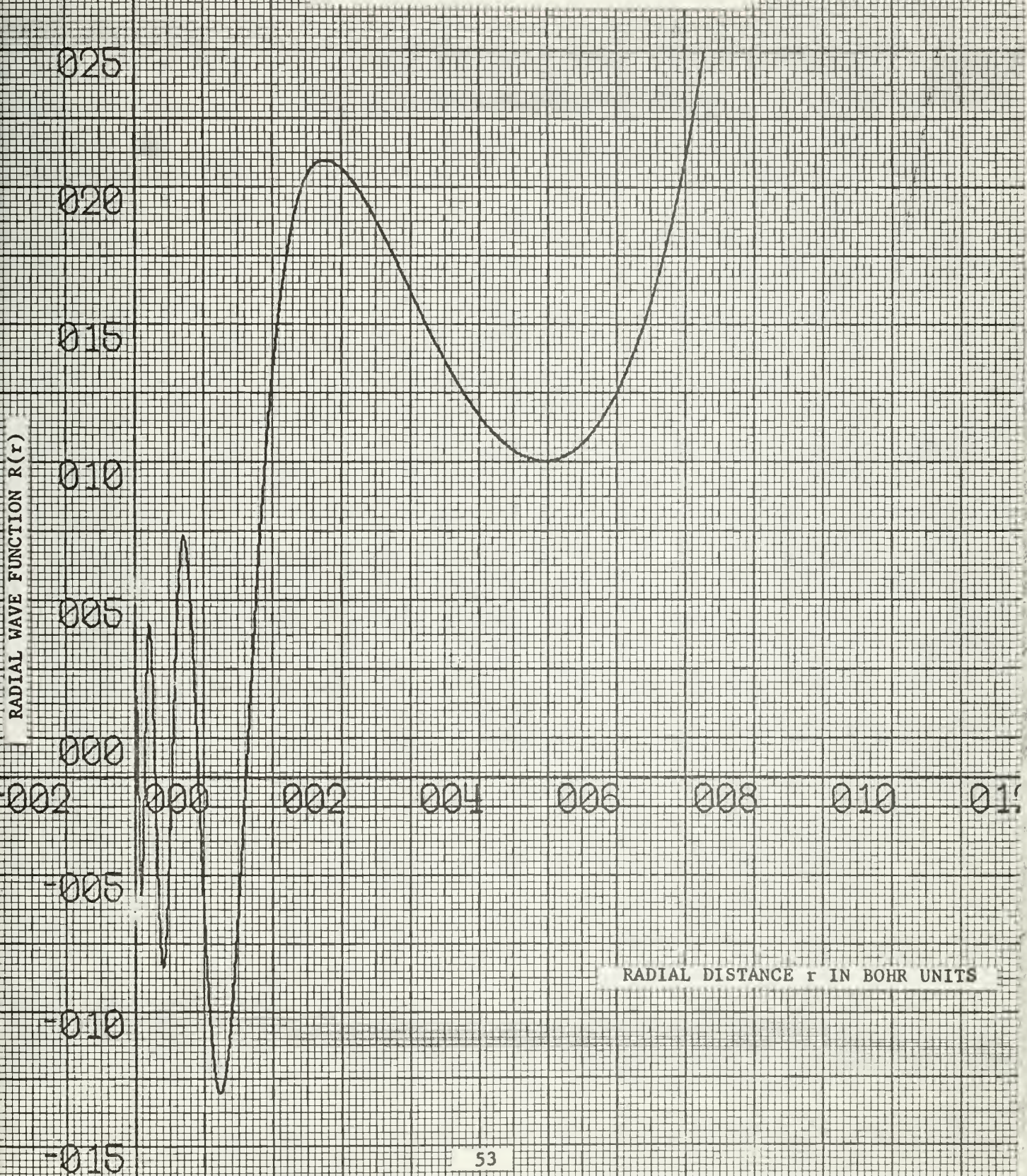
GOLD

RADIAL WAVE FUNCTION $R(r)$ vs.

RADIAL DISTANCE r

ENERGY STATE $E = .7$ RYDBERGS

RADIAL WAVE FUNCTION $R(r)$



RADIAL DISTANCE r IN BOHR UNITS

FIGURE 24
GOLD
RADIAL WAVE FUNCTION $R(r)$ vs.
RADIAL DISTANCE r
ENERGY STATE $E = .8$ RYDBERGS

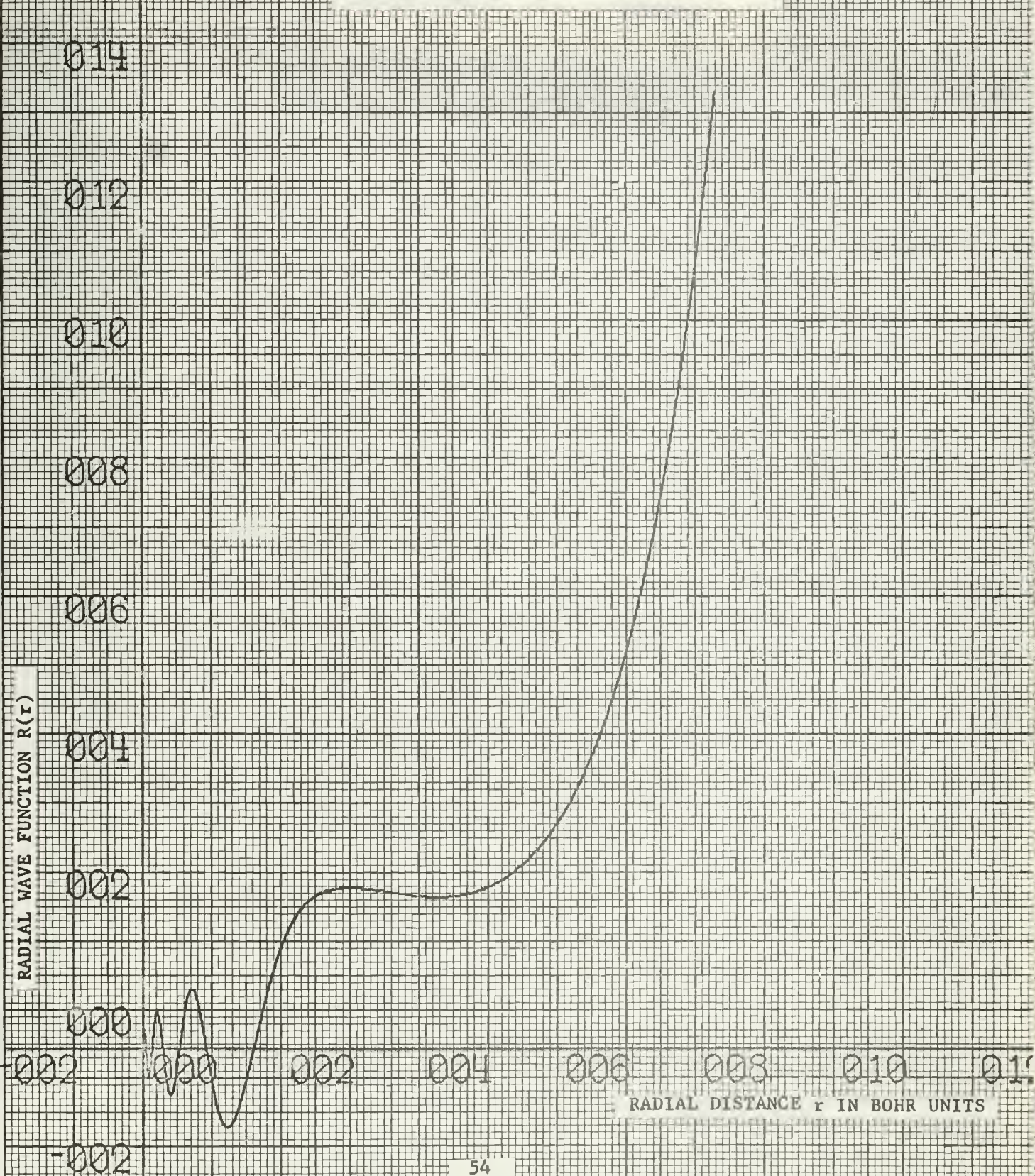


FIGURE 25

GOLD

RADIAL WAVE FUNCTION $R(r)$ vs.

RADIAL DISTANCE r

ENERGY STATE $E = .9$ RYDBERGS

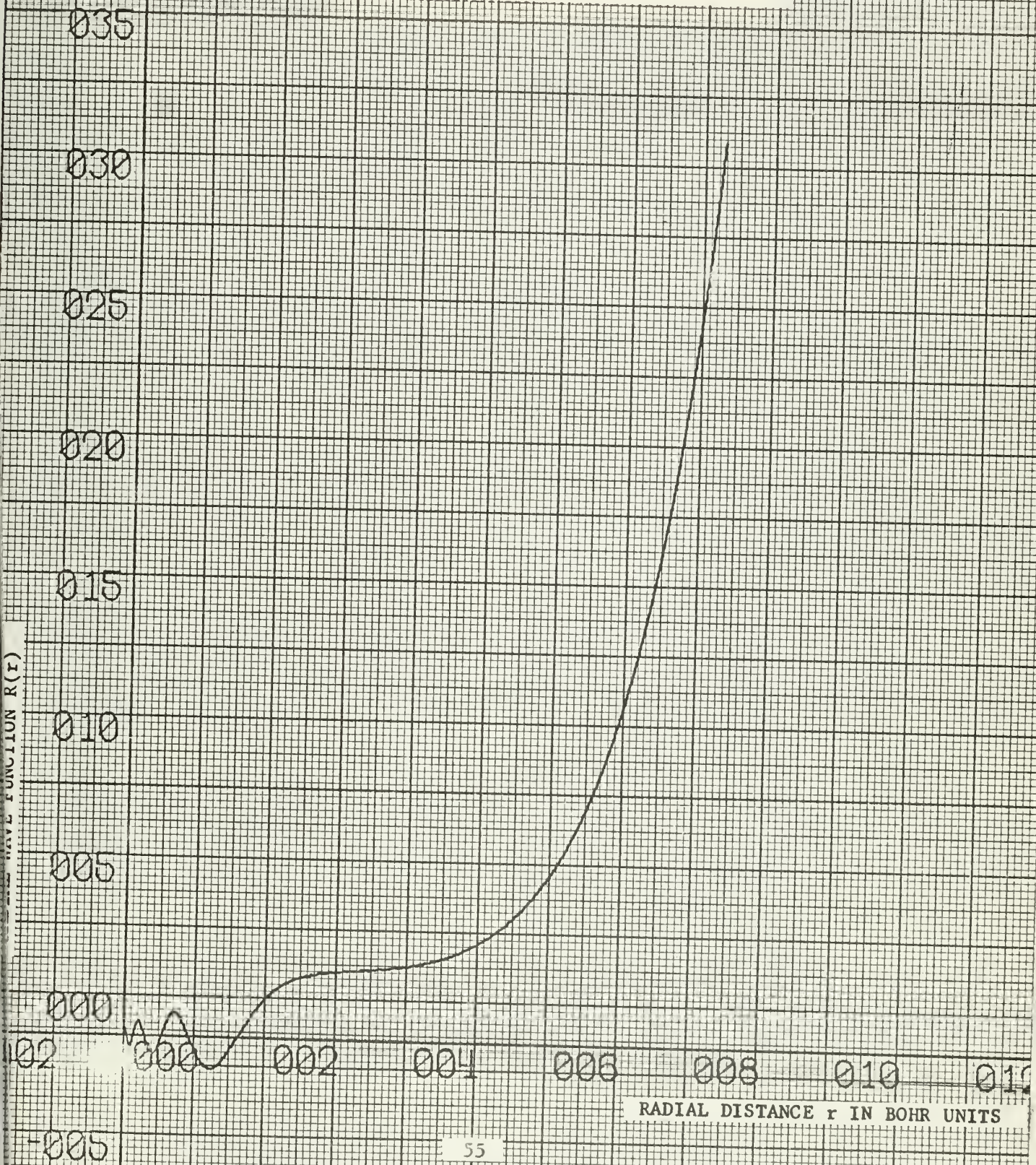


FIGURE 26
GOLD
RADIAL WAVE FUNCTION $R(r)$ vs.
RADIAL DISTANCE r
ENERGY STATE $E = 1.0$ RYDBERGS

RADIAL WAVE FUNCTION $R(r)$

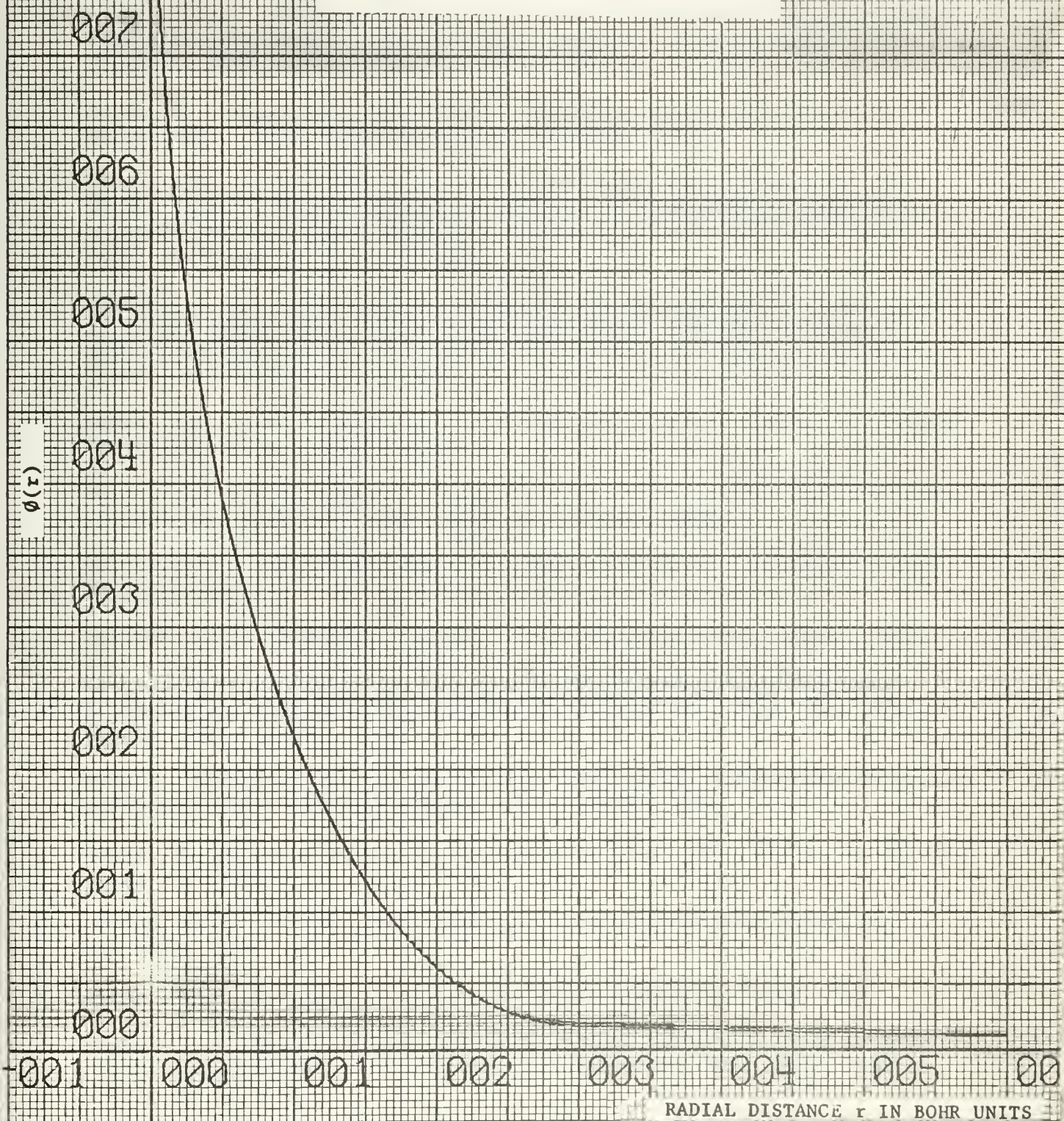
000

-002 000 002 004 006 008 010 012

-001

RADIAL DISTANCE r IN BOHR UNITS

FIGURE 27
GOLD
CONTRIBUTION TO THE EFFECTIVE
POTENTIAL $\phi(r)$ vs.
RADIAL DISTANCE r



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APPENDIX I

DEVELOPMENT OF A SERIES SOLUTION TO THE TRINOMIAL EQUATION

Basic Approach

The equation to be solved is in the form

$$\frac{d^2 R}{dr^2} + 2(V(r) - E)R = 0 \quad [I-1]$$

with $V(r) = \frac{Z \phi(r)}{r}$

Z = atomic number

$\phi(r)$ = known function of r

r = radius in units of Bohr radii

E = energy in units of $2 \times \text{Rydbergs} = 27 \text{ e.v}$

$\phi(r)$ decreases monotonically from

$$\phi(0) = 1.00 \text{ and approaches } 1/Z \text{ as } r \rightarrow \infty$$

Since $\phi(r)$ is given, the equation of a parabola through the points 0, 1, and 2 can be determined (Fig. 28a). The equation will be of the form $B + Qr + Tr^2$

Assume $\phi(r)$ is substituted into equation [I-1] and equation [I-1] is solved with suitable initial conditions. Then a solution is available in the range $0 \leq r \leq 2$ (Fig. 28b).

Calculate the values of $R(r)$ AT $r = 1$

$$\frac{dR(r)}{dr} \text{ AT } r = 1$$

Now pass a parabola through the points 1, 2 and 3, obtaining an approximation for the function $\phi(r)$ in this range. Then substitute the parabolic approximation into equation [I-1] using as initial conditions the previously calculated values of $R(r)$ and $\frac{dR(r)}{dr}$ at $r = 1$. The

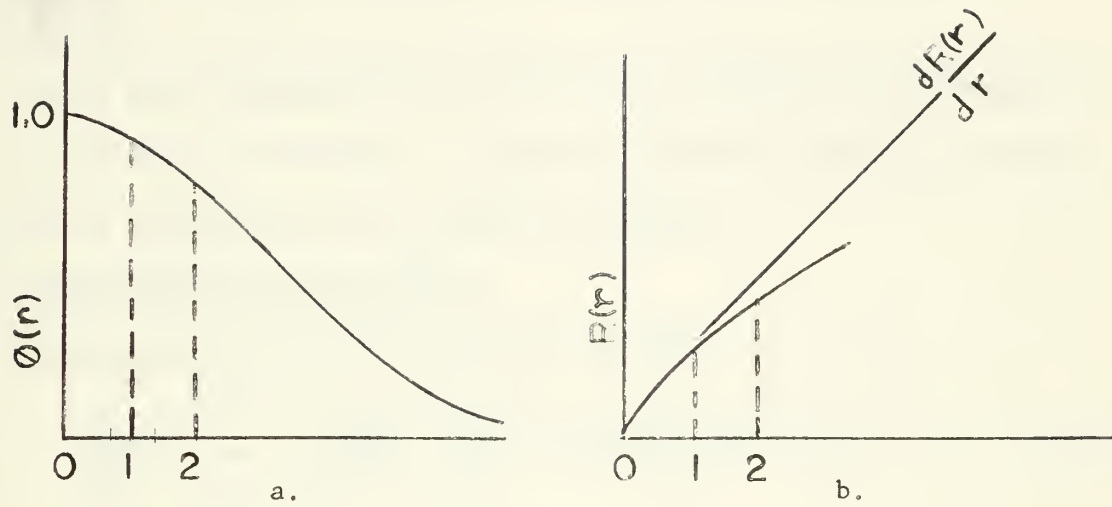


Fig. 28. The Boundary Value Approach.

solution now applies in range $1 < r < 5$. The values of $R(r)$ and $\frac{dR(r)}{dr}$ can now be calculated at midrange.

This process may now be continued as a series of boundary value problems until a complete solution is obtained. If the solution IS CONVERGENT IN EACH INTERVAL THE OVERALL SOLUTION IS CONVERGENT.

A very good approximation to the curve is obtained by evaluating at the half interval. Continuity of slope and position of $R(r)$ is assured since these values are used as initial conditions.

The Solution of the Equation

The equation [I-1] may be put into the form

$$\frac{d^2 R(r)}{dr^2} + \left(\frac{BB}{r} + QQ + RR \cdot r \right) R(r) = 0 \quad [I-2]$$

where

$$O(r) = B + Qr + Tr^2$$

$$BB = 2ZB$$

$$QQ = 2ZQ - 2E$$

$$RR = 2ZT$$

Let $r = e^\theta$ and multiply [I-2] by r^2

$$\left(\frac{r^2 d^2}{dr^2} + BB r + QQ r^2 + RR r^3 \right) R(r) = 0 \quad [I-3]$$

$$\frac{r^2 d^2}{dr^2} \text{ may be represented operationally as } D(D-1)$$

$$\frac{r^2 d^2}{dr^2} = D(D-1)$$

The solution of the equation $D(D-1)R(r) = 0$ is $R(r) = c_2 e^\theta + c_1$

²⁴G. Boole, op, cit.

Thus [I-3] may be written

$$\left(D(D-1) + BB e^{\theta} + QQ e^{2\theta} + RR e^{3\theta} \right) R(r) = 0$$

Operating on the left by $\frac{1}{D(D-1)}$

$$\left(1 + \phi_1(D) e^{\theta} + \phi_2(D) e^{2\theta} + \phi_3(D) e^{3\theta} \right) R(r) = C_1 + C_2 e^{\theta} \quad [I-4]$$

where

$$\phi_1(D) = \frac{BB}{D(D-1)}$$

$$\phi_2(D) = \frac{QQ}{D(D-1)}$$

$$\phi_3(D) = \frac{RR}{D(D-1)}$$

Operating on the left by

$$\left(1 + \phi_1(D) e^{\theta} + \phi_2(D) e^{2\theta} + \phi_3(D) e^{3\theta} \right)^{-1} = \Phi(D)^{-1}$$

$$R(r) = \Phi(D)^{-1} \{ C_1 + C_2 e^{\theta} \}$$

$\Phi(D)^{-1}$ may be expanded in the form

$$\sum_i F_i(D) e^{i\theta} = F_0(D) + F_1(D) e^{\theta} + F_2(D) e^{2\theta} + \dots + F_n(D) e^{n\theta}$$

then $\left(1 + \phi_1(D) e^{\theta} + \phi_2(D) e^{2\theta} + \phi_3(D) e^{3\theta} \right) \sum_i F_i(D) e^{i\theta} = 1$

The $F_i(D)$ may be evaluated in terms of $\phi_i(D)$ by equating like powers of $e^{n\theta}$ or $e^{i\theta}$

The relation

$$\phi_i(D) e^{n\theta} F_j(D) e^{m\theta} = \phi_i(D) F_j(D-n) e^{(n+m)\theta}$$

is required for the reduction.

Equating coefficients

$$\begin{aligned} F_0(D) &= 1 \\ F_1(D) &= -\phi_1(D) \\ F_2(D) &= -\phi_1(D) F_1(D-1) - \phi_2(D) \\ F_3(D) &= -\phi_1(D) F_2(D-1) - \phi_2(D) F_1(D-2) - \phi_3(D) \\ F_4(D) &= -\phi_1(D) F_3(D-1) - \phi_2(D) F_2(D-2) - \phi_3(D) F_1(D-3) \\ &\vdots \\ F_n(D) &= -\phi_1(D) F_{n-1}(D-1) - \phi_2(D) F_{n-2}(D-2) - \phi_3(D) F_{n-3}(D-3) \end{aligned}$$

The solution, once the F's are evaluated becomes

$$\begin{aligned} R(r) &= F_0(D) + F_1(D) e^\theta + F_2(D) e^{2\theta} + \dots + F_n(D) e^{n\theta} (C_1 + C_2 e^\theta) \\ &= C_1 (1 + F_1(D) e^\theta + F_2(D) e^{2\theta} + \dots + F_n(D) e^{n\theta}) \\ &\quad + C_2 (e^\theta + F_1(D) e^{2\theta} + F_2(D) e^{3\theta} + \dots + F_n(D) e^{(n+1)\theta}) \end{aligned}$$

[I-5]

The Starting Case

In this case the initial conditions are:

$$R(r) = 0 \quad r = 0 \quad [I-6]$$

$$\frac{dR(r)}{dr} = 1 \quad r = 0 \quad [I-7]$$

Equation [I-5] will be in the following form when the transformation of

$r = \frac{r}{a_0}$ is made.

$$R(r) = C_1(1 + G_1 r + G_2 r^2 + \dots) + C_2(r + F_1 r^2 + F_2 r^3 + \dots)$$

In order to satisfy the initial condition [I-6], C_1 must equal zero.

$$\frac{dR(r)}{dr} = C_2(1 + 2F_1 r + 3F_2 r^2 + \dots)$$

Thus when $r=0$ $\frac{dR(r)}{dr} = C_2$. The solution is thus some multiple of the slope. This multiple can be arbitrarily chosen. It is convenient to make the choice.

$$\frac{dR(r)}{dr} = 1, \quad r=0$$

Thus $R(r) = C^0 + F_1(r)C^{20} + F_2(r)C^{30} + \dots$

It now remains to evaluate the coefficients.

To determine B, Q and T

Given: $\phi(0) = 1$ $\phi(1)$ and $\phi(2)$

Let the interval be $h = 1/100$ Bohr Units

The equation $B + Qr + Tr^2$ must be satisfied at the three given points and $B = 1$

$$\phi(1) = B + Qh + Th^2$$

$$\phi(2) = B + 2Qh + 4Th^2$$

and Q and T may be determined.

For each given value of E the values of BB, QQ and RR are determined.

To Evaluate the Coefficients

Operationally

$$\frac{1}{f(D)} e^{n\theta} = \frac{e^{n\theta}}{f(r)}$$

provided $D-n$ is not a factor of $f(D)$

If $D-n$ is a factor $\Rightarrow f(D) = (D-n)g(D)$

$$\rightarrow \frac{1}{f(D)} e^{n\theta} = \frac{e^{n\theta}}{(D-n)g(D)} = \frac{e^{n\theta}}{(D-n)g(n)} = \frac{(\theta-1)e^{n\theta}}{g(n)}$$

$$\frac{1}{D-n} e^{n\theta} \text{ is the same as } (D-n)y = e^{n\theta}$$

$$D[(\theta-1)e^{n\theta}] = e^{n\theta} + n\theta e^{n\theta} - n e^{n\theta}$$

$$-n[(\theta-1)e^{n\theta}] = -n\theta e^{n\theta} + n e^{n\theta}$$

$$(D-n)[(\theta-1)e^{n\theta}] = e^{n\theta}$$

$$\frac{1}{D(D-1)} e^{n\theta} = \frac{1}{(D-1)(D-2)} e^{(n+1)\theta}$$

Thus, $F_1(D) e^{2\theta} = -\phi_1(D) e^{2\theta}$

$$= -\frac{BB}{D(D-1)} e^{2\theta}$$

$$= -\frac{BB}{2} e^{2\theta}$$

Let $-\frac{BB}{2} = F_1(2)$

Similarly,

$$F_2(D)e^{3\theta} = -(\phi_1(D)F_1(D-1) + \phi_2(D))e^{3\theta}$$

$$F_1(D-1)e^{3\theta} = F_1(D)e^{2\theta}$$

$$F_1(D-1) = F_1(2)$$

$$\rightarrow F_2(D)e^{3\theta} = -\left(\frac{BB}{D(D-1)}F_1(2) - \frac{QQ}{D(D-1)}\right)e^{3\theta}$$

$$\text{Let } -\frac{1}{3 \cdot 2}(-BB F_1(2) - QQ) = F_2(3)$$

$$\begin{aligned} F_3(D)e^{4\theta} &= -(\phi_1(D)F_2(D-1) - \phi_2(D)F_1(D-2) - \phi_3(D))e^{4\theta} \\ &= -\left(\frac{BB}{D(D-1)}F_2(3) - \frac{QQ}{D(D-1)}F_1(2) - \frac{RR}{D(D-1)}\right)e^{4\theta} \end{aligned}$$

$$\text{Let } -\frac{1}{4 \cdot 3}(BB F_2(3) - QQ F_1(2) - RR) = F_3(4)$$

$$F_4(D)e^{5\theta} = -\left(\frac{BB}{D(D-1)}F_3(4) - \frac{QQ}{D(D-1)}F_2(3) - \frac{RR}{D(D-1)}F_1(2)\right)e^{5\theta}$$

$$\text{Let } -\frac{1}{5 \cdot 4}(BB F_3(4) - QQ F_2(3) - RR F_1(2)) = F_4(5)$$

In general

$$F_n(n+1) = -\frac{1}{n(n-1)}\left\{BB F_{n-1}(n-1) + QQ F_{n-2}(n-2) + RR F_{n-3}(n-3)\right\}$$

This type of recursion formula is easily put in FORTRAN language and the number of coefficients that can be calculated is unlimited.

Using the notation $F_n(n+1) = F_n$

$$R(r) = e^{\theta} + F_1 e^{2\theta} + F_2 e^{3\theta} + \dots + F_n e^{(n+1)\theta}$$

or since $r = e^{\theta}$ the equation becomes

$$R(r) = r + F_1 r^2 + F_2 r^3 + F_3 r^4 + \dots + F_n r^{n+1} \quad [I-8]$$

This equation is easily summed in FORTRAN language. The convergence is most easily observed by calculating the partial sums. For the initial calculation with $h = .01$ it was observed that ten terms were sufficient to reach the limit of the machine 10^{-307} . Equation [I-8] was used to compute the starting values of all computations.

The Case When the Initial Conditions Are:

$$R(r) = R(k) \quad r = k$$

$$\frac{dR(r)}{dr} = R'(k) \quad r = k$$

The form of the equations will be

$$\begin{aligned} R(r) &= C_1 (1 + G_1 r + G_2 r^2 + \dots + G_n r^n) \\ &\quad + C_2 (r + F_1 r^2 + F_2 r^3 + \dots + F_n r^{n+1}) \\ \frac{dR(r)}{dr} &= C_1 (G_1 + 2G_2 r + 3G_3 r^2 + \dots + nG_n r^{n-1}) \\ &\quad + C_1 \left(r \frac{dG_1}{dr} + r^2 \frac{dG_2}{dr} + \dots + r^n \frac{dG_n}{dr} \right) \\ &\quad + C_2 (1 + 2F_1 r + 3F_2 r^2 + \dots + nF_n r^{n-1}) \end{aligned}$$

It will be shown that G_i is a function of r and F_i is a constant.

At any coordinate $r=k$ if $G_1, \frac{dG_1}{dr}$ and F_2 are determined.

Then

$$R(k) = C_1 g_1(k) + C_2 f_1(k)$$

$$R'(k) = C_1 g_2(k) + C_2 f_2(k)$$

Thus C_1 and C_2 are determined.

For the portion

$$R(\omega) = C_2 (e^{\theta} + F_1(\omega) e^{2\theta} + \dots + F_n(\omega) e^{(n+1)\theta})$$

the solution is exactly the same as the starting case.

For

$$R(\omega) = C_1 (1 + G_1(\omega) e^{\theta} + G_2(\omega) e^{2\theta} + \dots + G_n(\omega) e^{n\theta})$$

the calculation is more complex.

$$\begin{aligned} F_1(\omega) e^{\theta} &= -\phi_1(\omega) e^{\theta} \\ &= -\frac{BB}{D(D-1)} e^{\theta} \\ &= -BB(\theta-1) e^{\theta} \end{aligned}$$

Now change to the following rather complex notation. This notation will be needed later when derivatives are taken.

Since $r = e^{\theta}$ $\theta = \ln r$

Let

$$\begin{aligned} V(1) &= -BB \\ AC(1) &= V(1) \\ VV(1) &= BB \\ BC(1) &= VV(1) \\ G(1) &= AC(1)\theta + BC(1) \end{aligned}$$

Then $F(D)e^{\theta} = G(1)e^{\theta}$

$$\frac{1}{D(D-1)} \theta e^{n\theta} = e^{n\theta} \left\{ \frac{1}{n+D(D+n-1)} \theta \right\}$$

$$(D+n)(D+n-1) = D^2 + (2n-1)D + n(n-1)$$

$$= n(n+1) \left\{ 1 + \frac{2n-1}{n(n+1)} D + \frac{D^2}{n(n+1)} \right\}$$

Since $D^2\theta = 0$ dividing the remainder into one,

$$1 + \frac{2n-1}{n(n+1)} D \sqrt{1} = 1 - \frac{2n-1}{n(n+1)} D$$

Thus $\frac{1}{D(D-1)} \theta e^{n\theta} = e^{n\theta} \left\{ \frac{1}{n(n+1)} - \frac{(2n-1)}{(n(n+1))^2} D \right\} \theta$

$$= \frac{e^{n\theta}}{n(n+1)} \left\{ \theta - \frac{2n-1}{n(n+1)} \right\} \quad n \geq 2$$

Evaluating $F_2(D)$

$$\begin{aligned} F_2(D) e^{2\theta} &= -\phi_1(D) F_1(D-1) e^{2\theta} - \phi_2(D) e^{2\theta} \\ &= -\frac{BB}{D(D-1)} AC(1) \theta e^{2\theta} - \frac{BB}{D(D-1)} BC(1) e^{2\theta} - \frac{QQ}{D(D-1)} e^{2\theta} \end{aligned}$$

$$= - \left(\frac{BB}{2} \left(\theta - \frac{3}{2} \right) AC(1) + \frac{BB}{2} BC(1) + \frac{QQ}{2} \right) e^{2\theta}$$

$$V(2) = -\frac{BB \cdot AC(1)}{2}$$

$$VV(2) = -\frac{BB}{2} \left(BC(1) - \frac{3}{2} AC(1) \right)$$

$$WW(2) = -\frac{QQ}{2}$$

$$AC(2) = V(2)$$

$$BC(2) = VV(2) + WW(2)$$

$$G(2) = AC(2) \theta + BC(2)$$

Proceeding in like manner for $F_3(D)$

$$V(3) = -\frac{BB}{6} AC(2) \quad VV(3) = -\frac{1}{6} \left\{ \frac{5BB}{6} AC(2) + BC(2) \right\}$$

$$W(3) = -\frac{QQ}{6} AC(1) \quad WW(3) = -\frac{1}{6} \left\{ \frac{5QQ}{6} AC(1) + BC(1) \right\}$$

$$XX(3) = -\frac{1}{6} \cdot RR$$

$$AC(3) = V(3) + W(3) \quad BC(3) = VV(3) + WW(3) + XX(3)$$

$$G(3) = AC(3) \cdot \theta + BC(3)$$

The General Term becomes

$$V(J) = -\frac{1}{J(J+1)} (BB \cdot AC(J-1))$$

$$W(J) = -\frac{1}{J(J+1)} (QQ \cdot AC(J-2))$$

$$X(J) = -\frac{1}{J(J+1)} (RR \cdot AC(J-3))$$

$$VV(J) = -\frac{1}{J(J+1)} (BB \cdot AC(J-1) \left(\frac{2J-1}{J(J-1)} \right) + BC(J-1))$$

$$WW(J) = -\frac{1}{J(J+1)} (QQ \cdot AC(J-2) \left(\frac{2J-1}{J(J-1)} \right) + BC(J-2))$$

$$XX(J) = -\frac{1}{J(J+1)} (RR \cdot AC(J-3) \left(\frac{2J-1}{J(J-1)} \right) + BC(J-3))$$

$$AC(J) = V(J) + W(J) + X(J)$$

$$BC(J) = VV(J) + WW(J) + XX(J)$$

$$G(J) = AC(J) \cdot \theta + BC(J)$$

For example

$$G(4) = AC(4) \cdot \theta + BC(4)$$

$$BC(4) = VV(4) + WW(4) + XX(4)$$

Thus $VV(4) = -\frac{1}{4 \cdot 3} (BB \cdot AC(3) \cdot \frac{7}{12} + BC(3))$

Therefore the form of the equation will be

$$R(r) = C_1 (1 + G_1 \theta^0 + G_2 \theta^{20} + \dots + G_n \theta^{n0})$$

since $r = \theta^0$, $G_i = AC(i) \theta + BC(i) = AC(i) \ln r + BC(i)$

$$R(r) = C_1 (1 + \ln r [AC(1) \cdot r + AC(2) \cdot r^2 + \dots]) + C_1 (BC(1) \cdot r + BC(2) \cdot r^2 + BC(3) \cdot r^3 + \dots)$$

and the complete solution is

$$R(r) = C_1 (1 + \ln r [AC(1) \cdot r + AC(2) \cdot r^2 + \dots]) + C_1 (BC(1) \cdot r + BC(2) \cdot r^2 + \dots) + C_2 (r + F_1 r^2 + F_2 r^3 + \dots)$$

$$\begin{aligned} \frac{dR(r)}{dr} = & C_1 \left\{ \frac{1}{r} (AC(1) \cdot r + AC(2) \cdot r^2 + \dots - AC(n) \cdot r^n) \right\} \\ & + C_1 \left\{ \ln r (AC(1) + 2AC(2) \cdot r + \dots - nAC(n) r^{n-1}) \right\} \\ & + C_1 \left\{ BC(1) + 2BC(2) \cdot r + \dots - nBC(n) r^{n-1} \right\} \\ & + C_2 \left\{ 1 + 2F_1 r + 3F_2 r^2 + \dots - nF_{n-1} r^{n-1} \right\} \end{aligned}$$

A similar expression can be derived for the second derivative.

Discussion of the Equation

The equation of $R(r)$ is slowly converging. The second derivative is more slowly converging. The self-checking feature is obtained by comparing the second derivative with the value of the second derivative calculated from

$$\frac{d^2 R}{dr^2} = f(r) R$$

It was observed that 10 terms of the series were sufficient to tax the limit of machine accuracy for the starting values. When $r = 1$ the number of terms required is 25, 50 for $r = 3$, and 75 for $r = 8$.

The number of calculations required to carry out the series to 75 terms is fantastic. One run required 20 minutes of machine time. In order to determine the lowest energy state and to properly determine the points of tangency, increments of .001 E were used. Thus it would take approximately 30 machine hours to complete one Wigner-Seitz calculation using this method.

Even though the 75th coefficient time $(8)^{75}$ was of the order of 10^{-200} the build-up errors encountered because of the large number of calculations allowed agreement on the check to only 10^{-8} .

The equation did, however, serve its purpose and enabled us to establish a criterion. Fortunately the simplest formula used

$$R(r+\Delta r) = (2 - (\Delta r)^2 f(r)) R(r) - R(r-\Delta r)$$

using an interval of .01 Bohr units duplicated the results of the very complex system described above to 10^{-6} . The Wigner-Seitz calculation by this method takes approximately 5 to 10 minutes of machine time compared with 30 hours for the complex method.

APPENDIX II

THE RADIAL WAVE FUNCTIONS $R(r)$ FOR ENERGIES RANGING FROM THE IONIZATION ENERGY TO THE LOWEST ENERGY STATE FOR COPPER, SILVER, AND GOLD.

FIGURE 29
COPPER - HARTREE-FOCK
CONTRIBUTIONS TO THE EFFECTIVE
POTENTIAL $\phi(r)$ vs.
RADIAL DISTANCE r

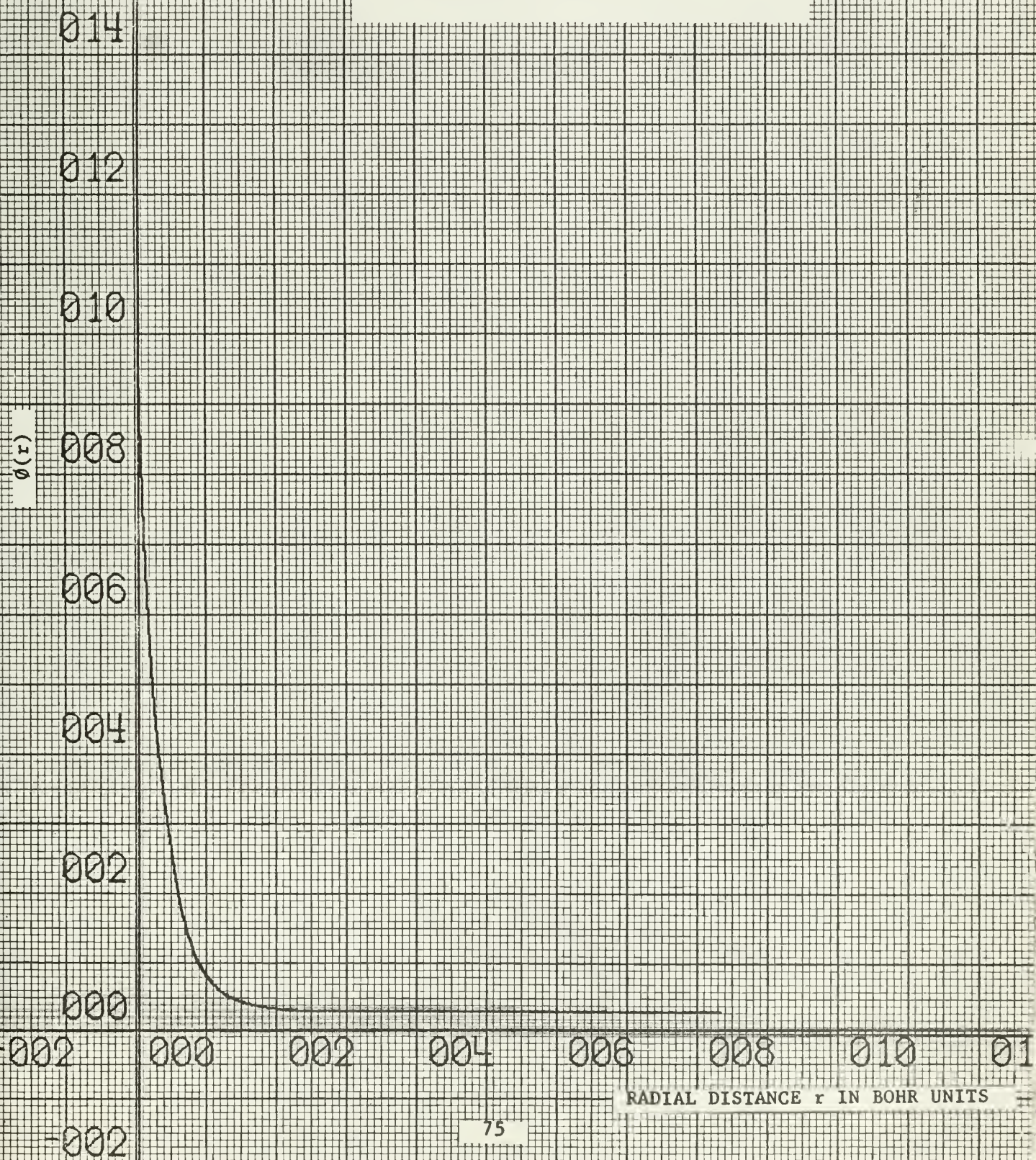


FIGURE 30

COPPER

RADIAL WAVE FUNCTION $R(r)$ vs.

RADIAL DISTANCE r

HARTREE-FOCK POTENTIAL

ENERGY STATE $E = .32$ RYDBERGS

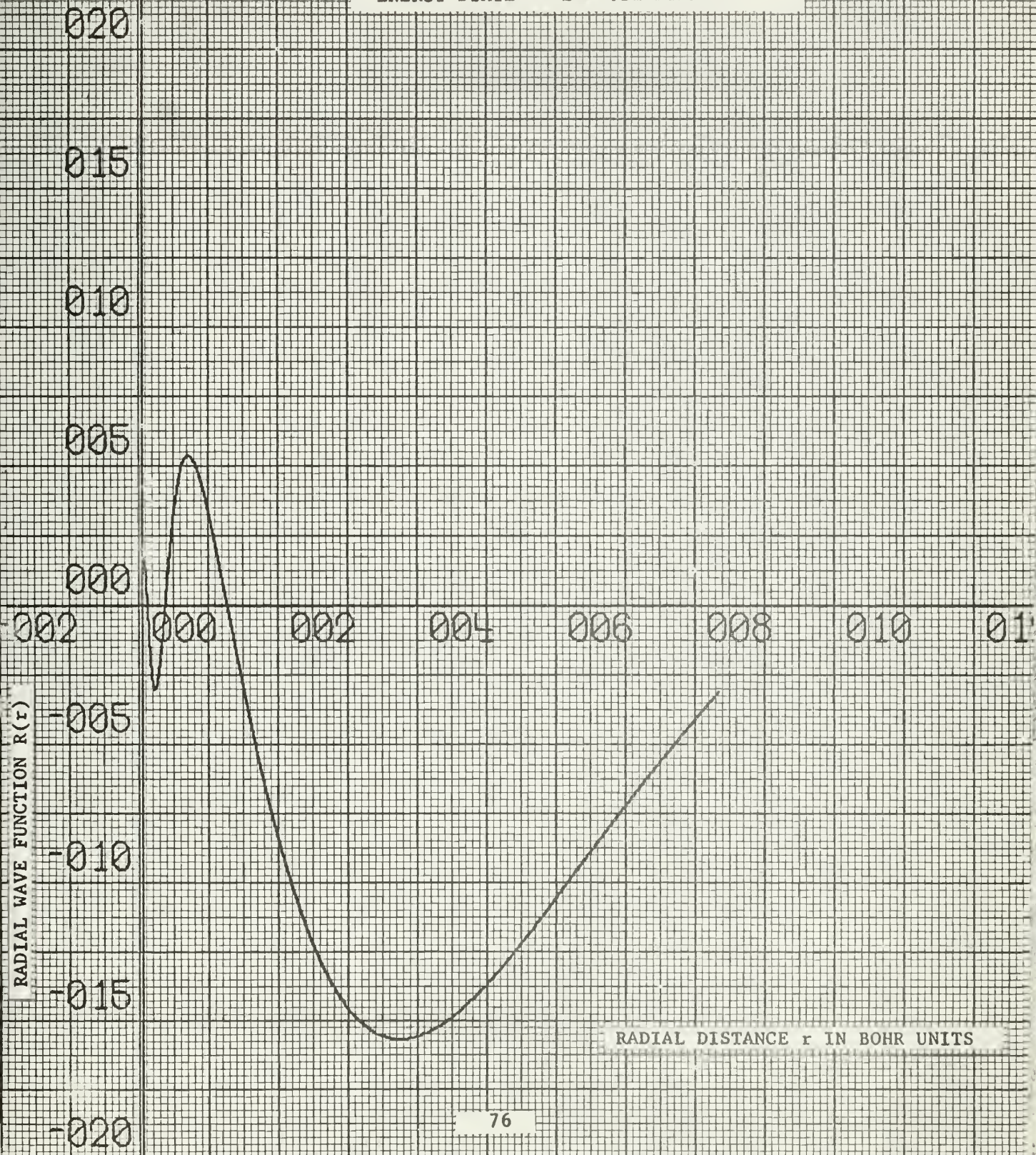


FIGURE 31

COPPER

RADIAL WAVE FUNCTION $R(r)$ vs.

RADIAL DISTANCE r

HARTREE-FOCK POTENTIAL

ENERGY STATE $E = .34$ RYDBERGS

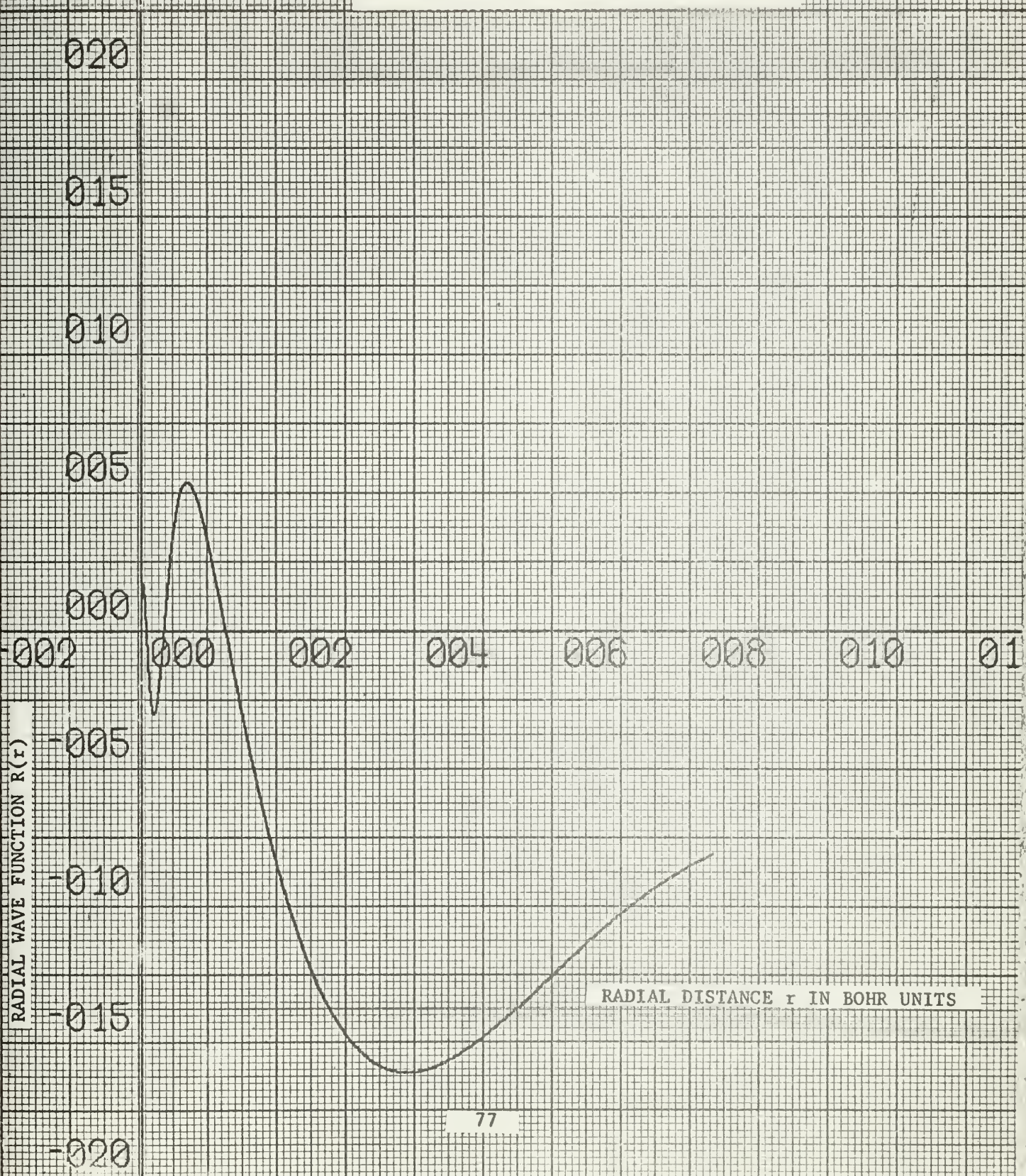


FIGURE 32

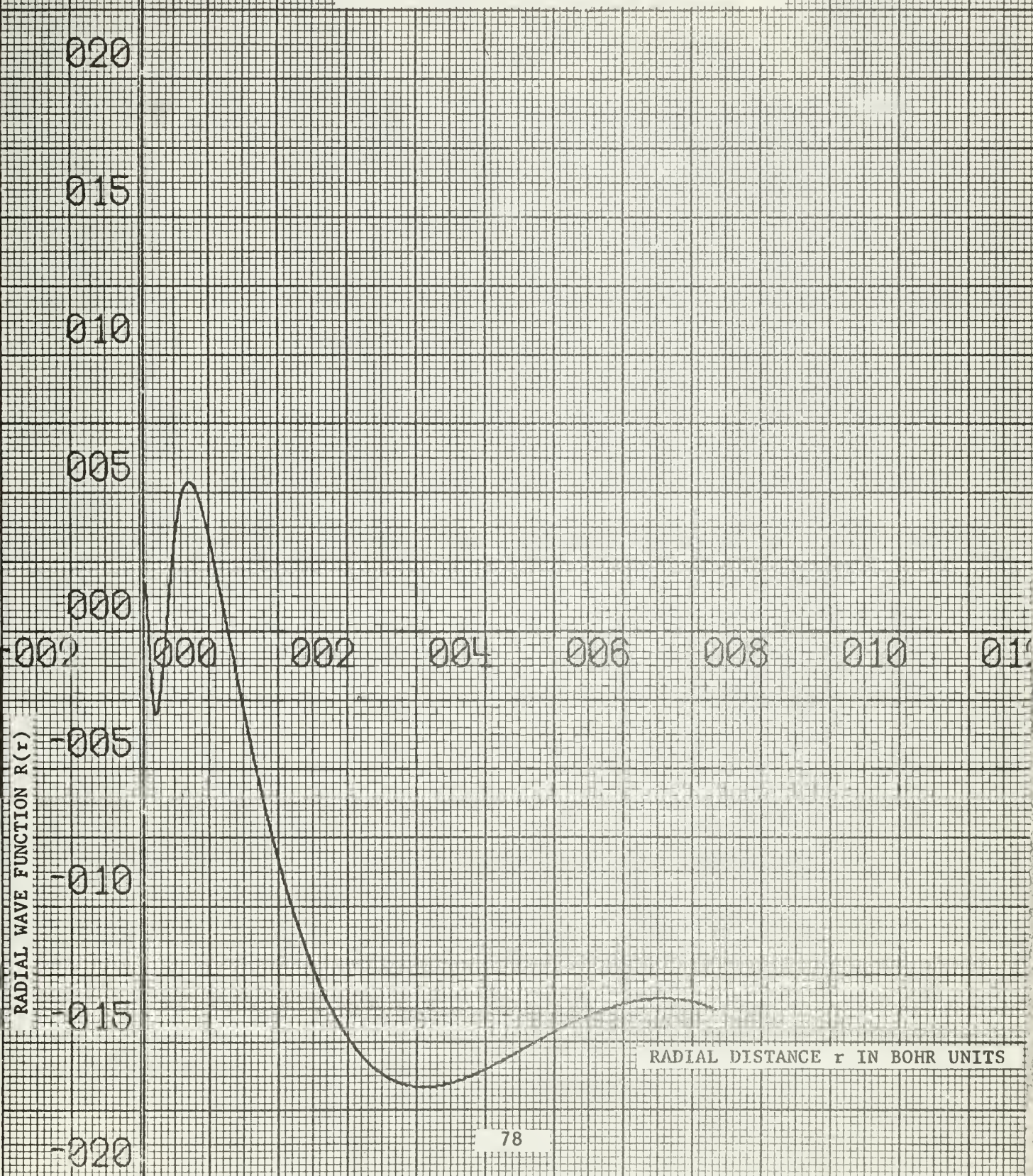
COPPER

RADIAL WAVE FUNCTION $R(r)$ vs.

RADIAL DISTANCE r

HARTREE-FOCK POTENTIAL

ENERGY STATE $E = .36$ RYDBERGS



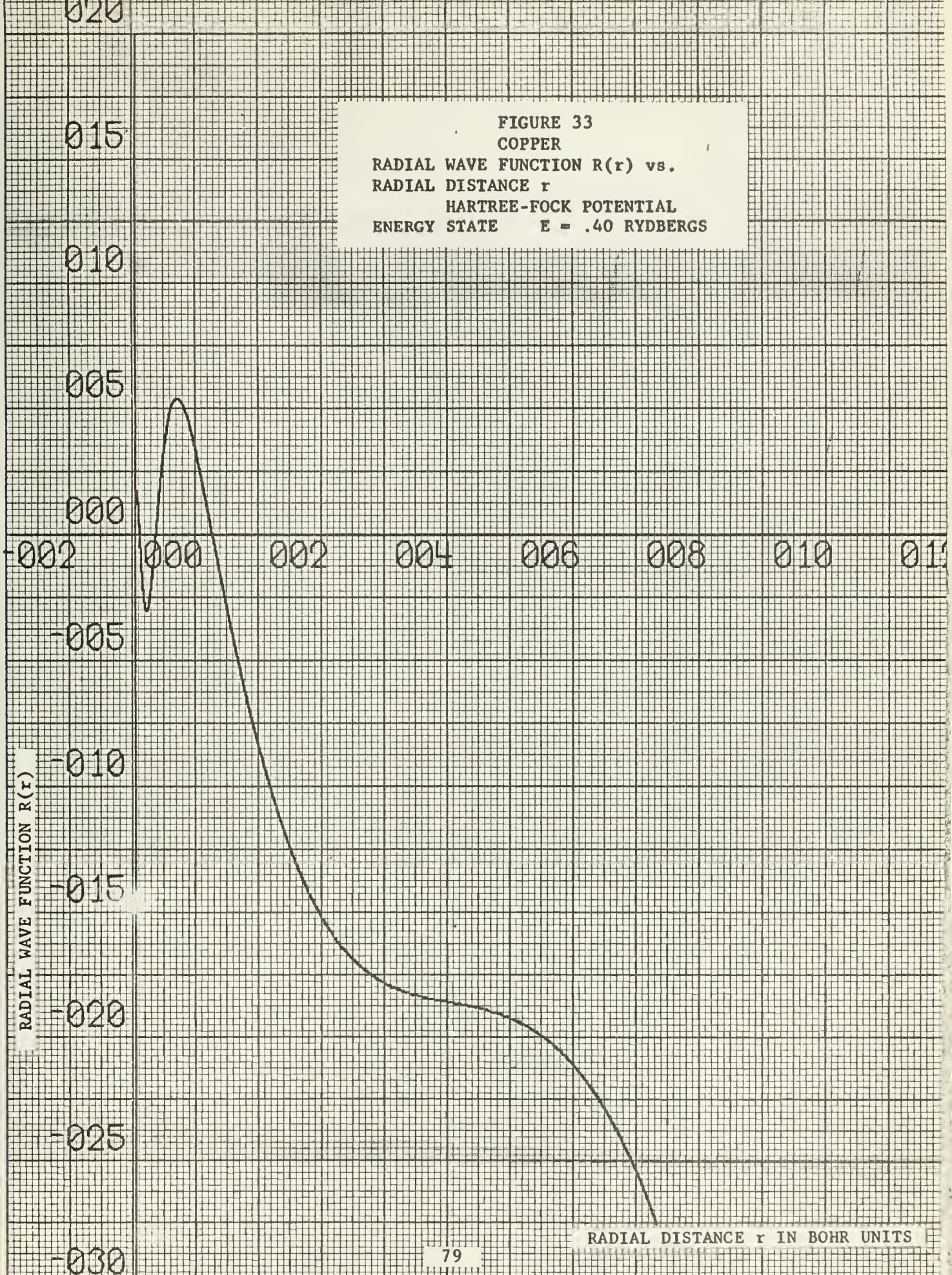


FIGURE 34

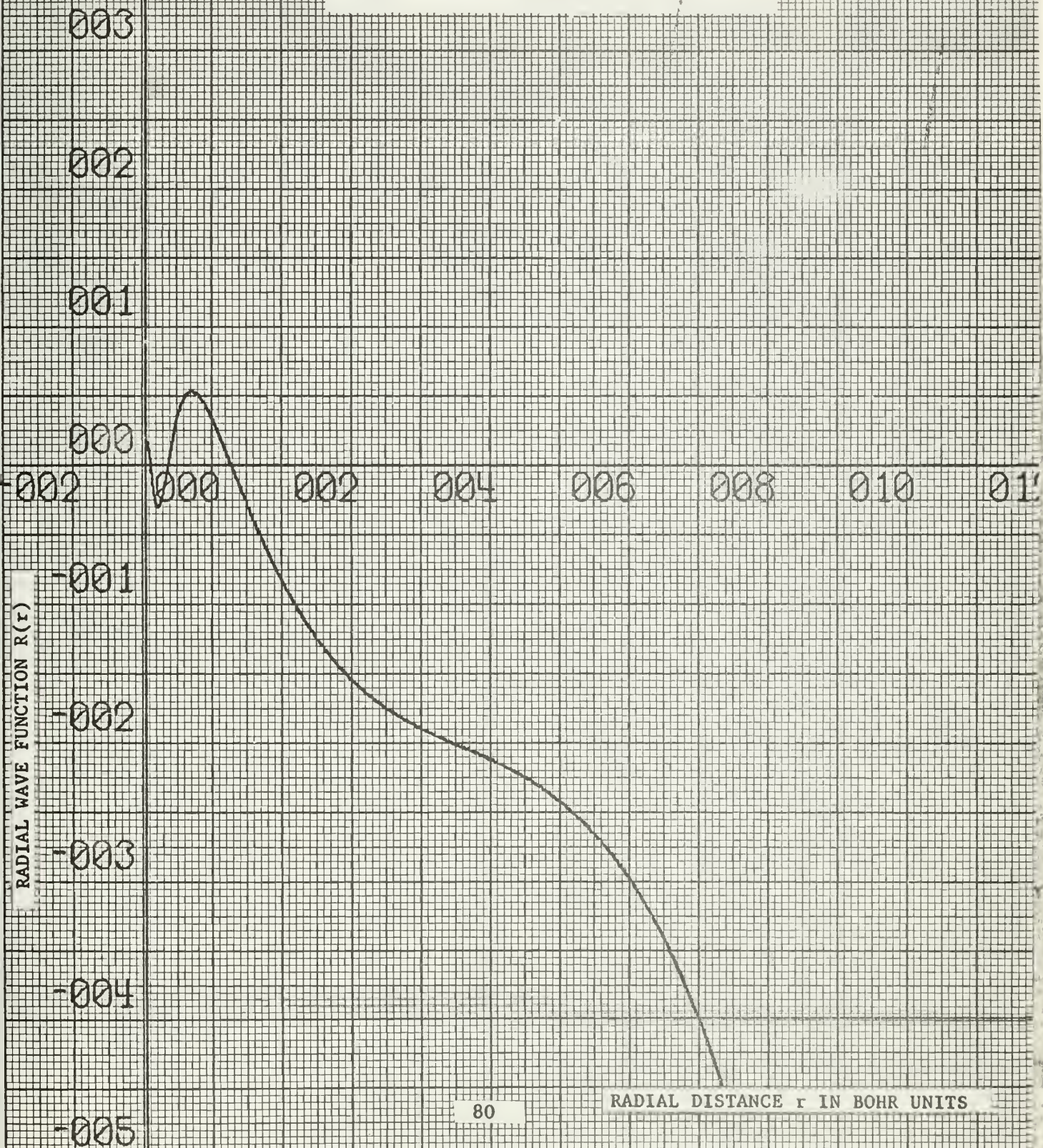
COPPER

RADIAL WAVE FUNCTION $R(r)$ vs.

RADIAL DISTANCE r

HARTREE-FOCK POTENTIAL

ENERGY STATE $E = .44$ RYDBERGS



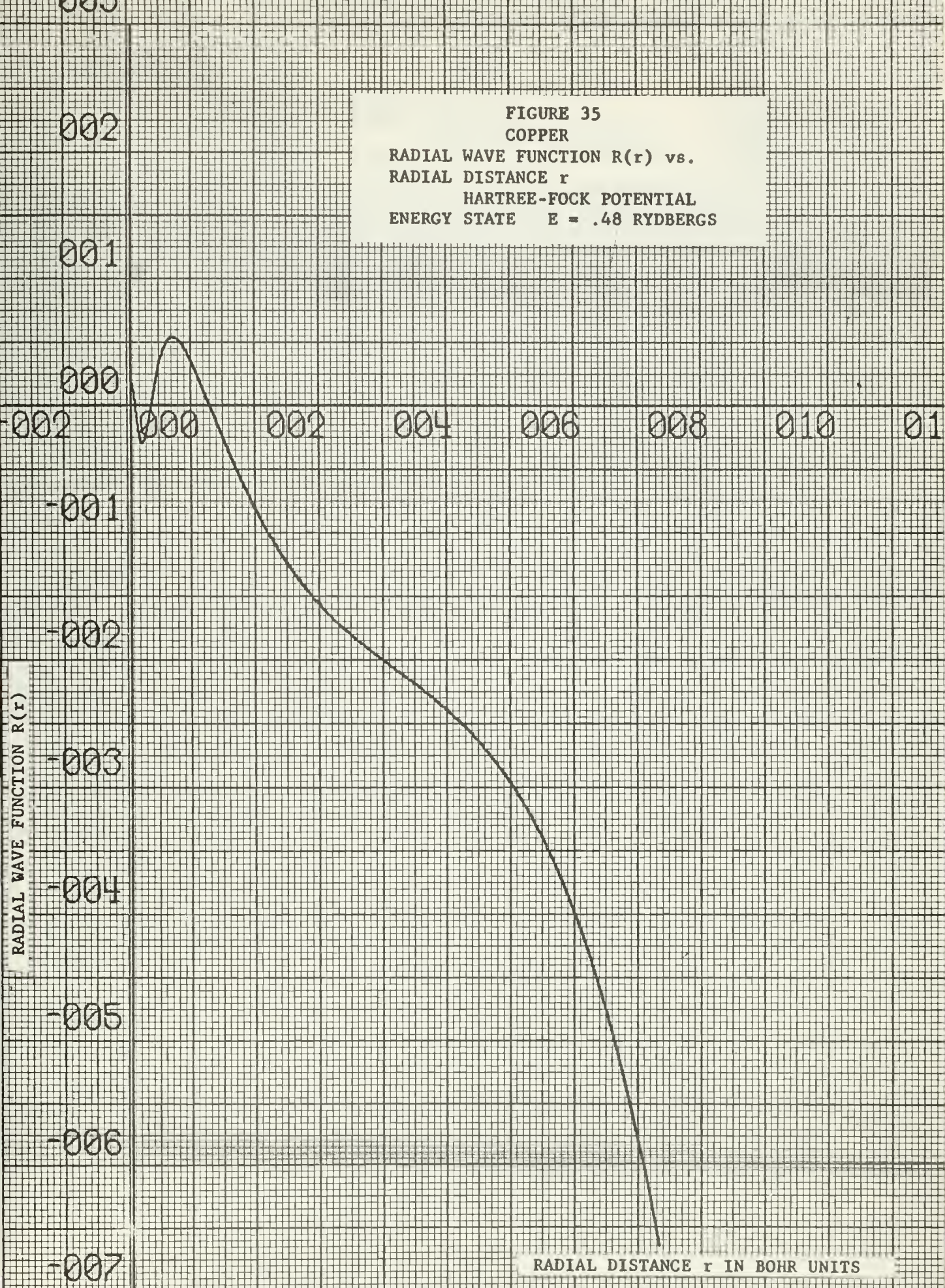


FIGURE 36
COPPER
RADIAL WAVE FUNCTION $R(r)$ vs.
RADIAL DISTANCE r
HARTREE-FOCK POTENTIAL
ENERGY STATE $E = .52$ RYDBERGS

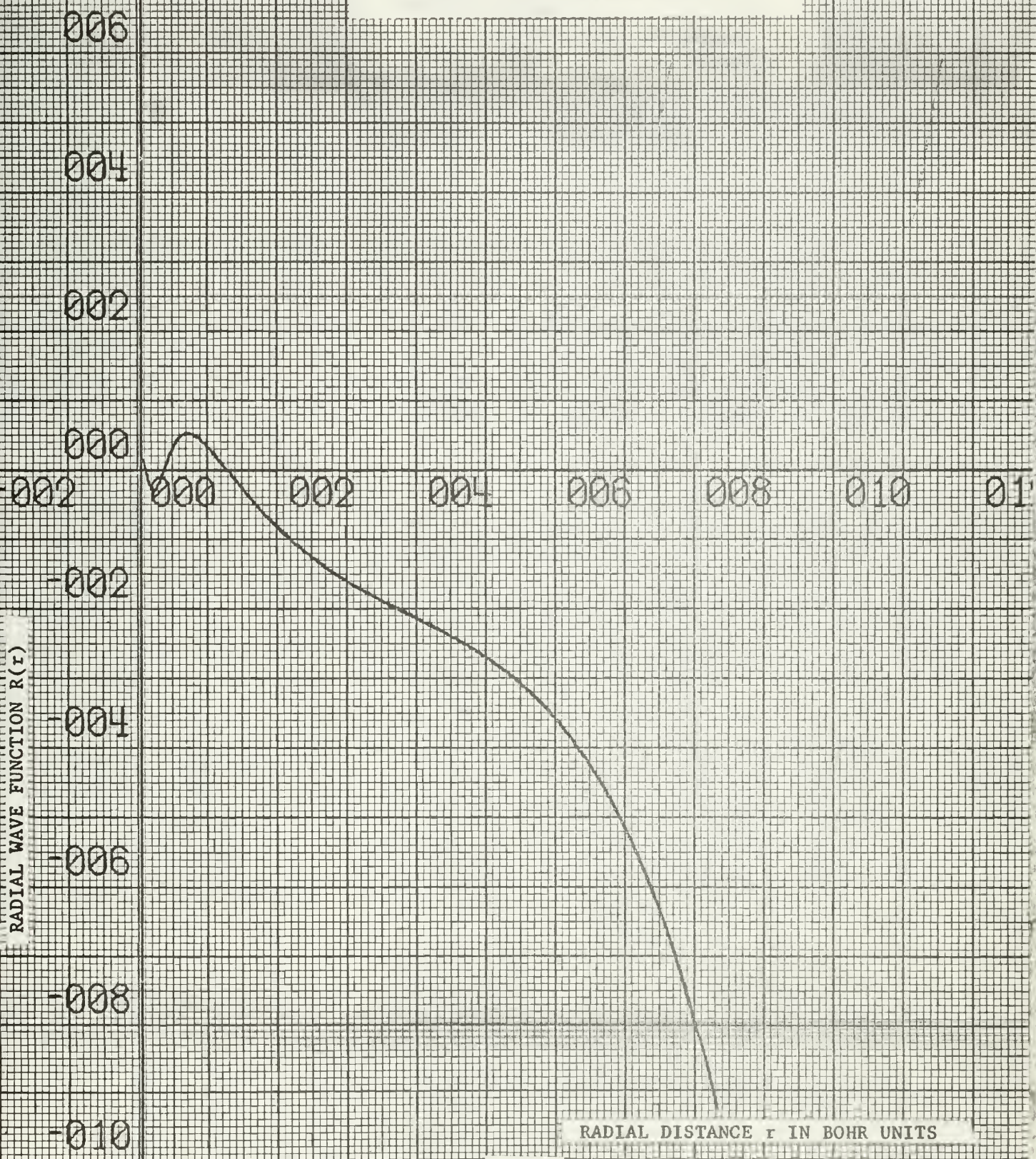


FIGURE 37
COPPER
RADIAL WAVE FUNCTION $R(r)$ vs.
RADIAL DISTANCE r
HARTREE-FOCK POTENTIAL
ENERGY STATE $E = .53$ RYDBERGS

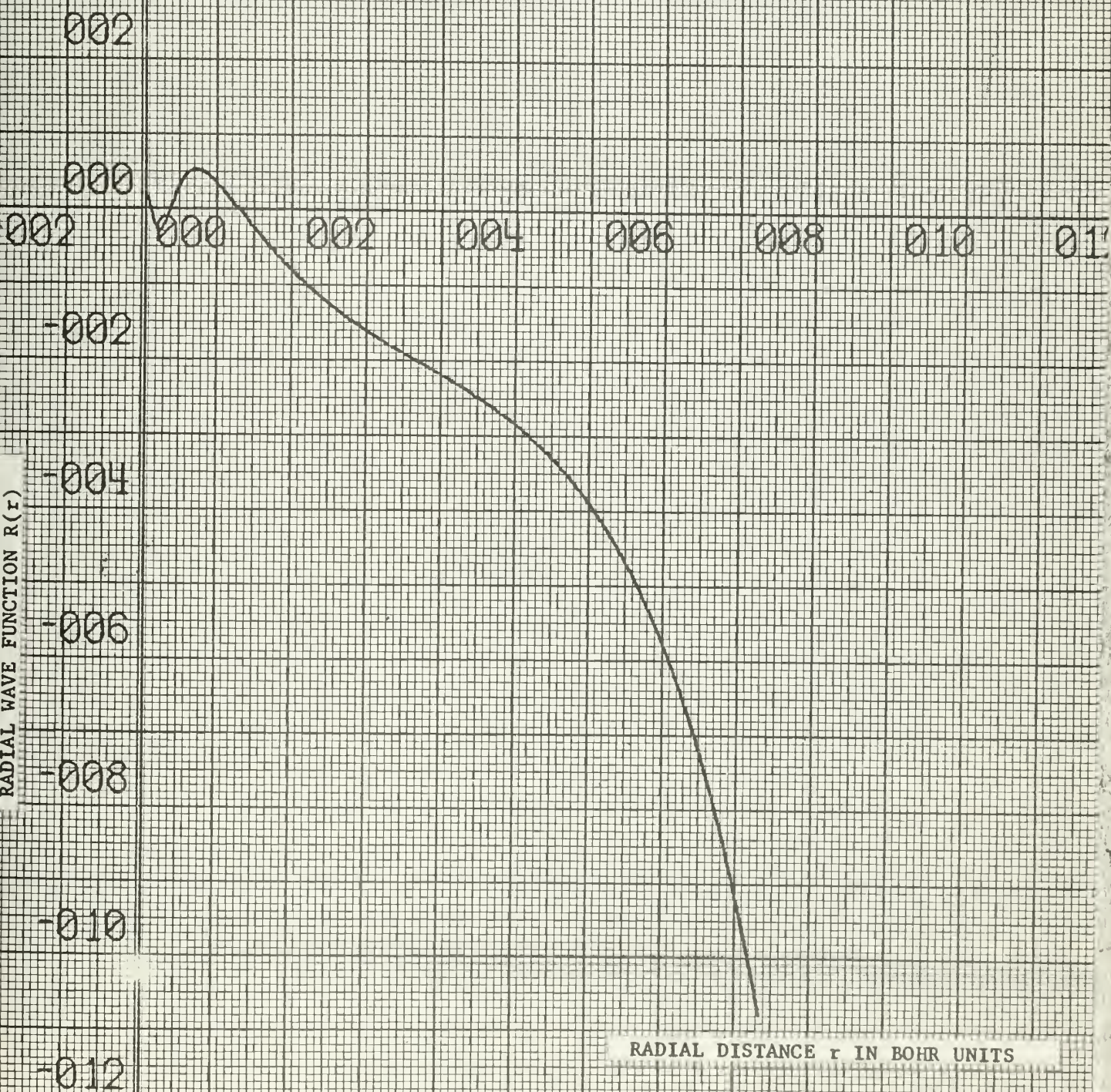


FIGURE 38
COPPER
RADIAL WAVE FUNCTION $R(r)$ vs.
RADIAL DISTANCE r
HARTREE-FOCK POTENTIAL
ENERGY STATE $E = .54$ RYDBERGS

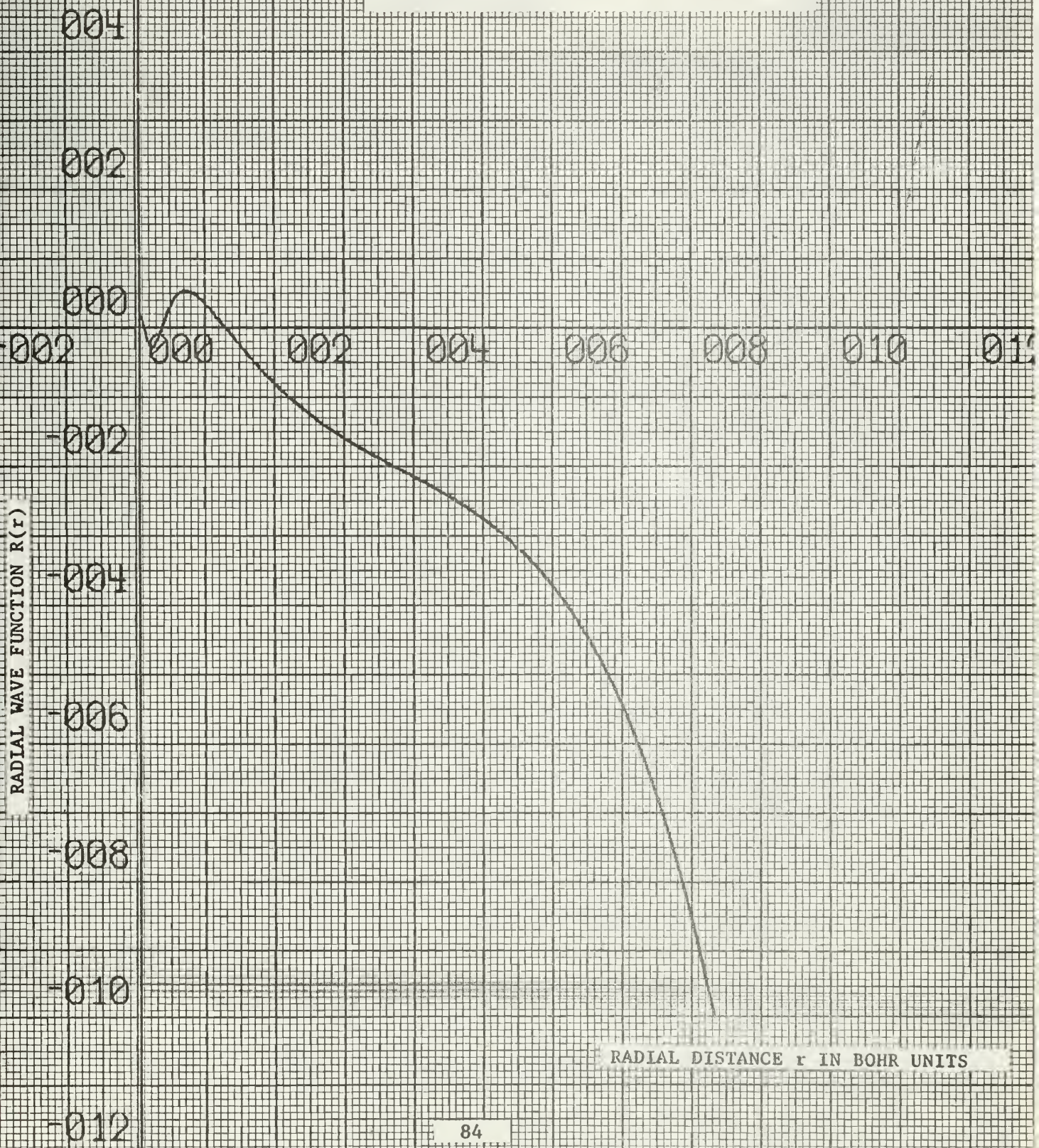


FIGURE 39
COPPER - THOMAS-FERMI
CONTRIBUTIONS TO THE EFFECTIVE
POTENTIAL $\phi(r)$ vs.
RADIAL DISTANCE r

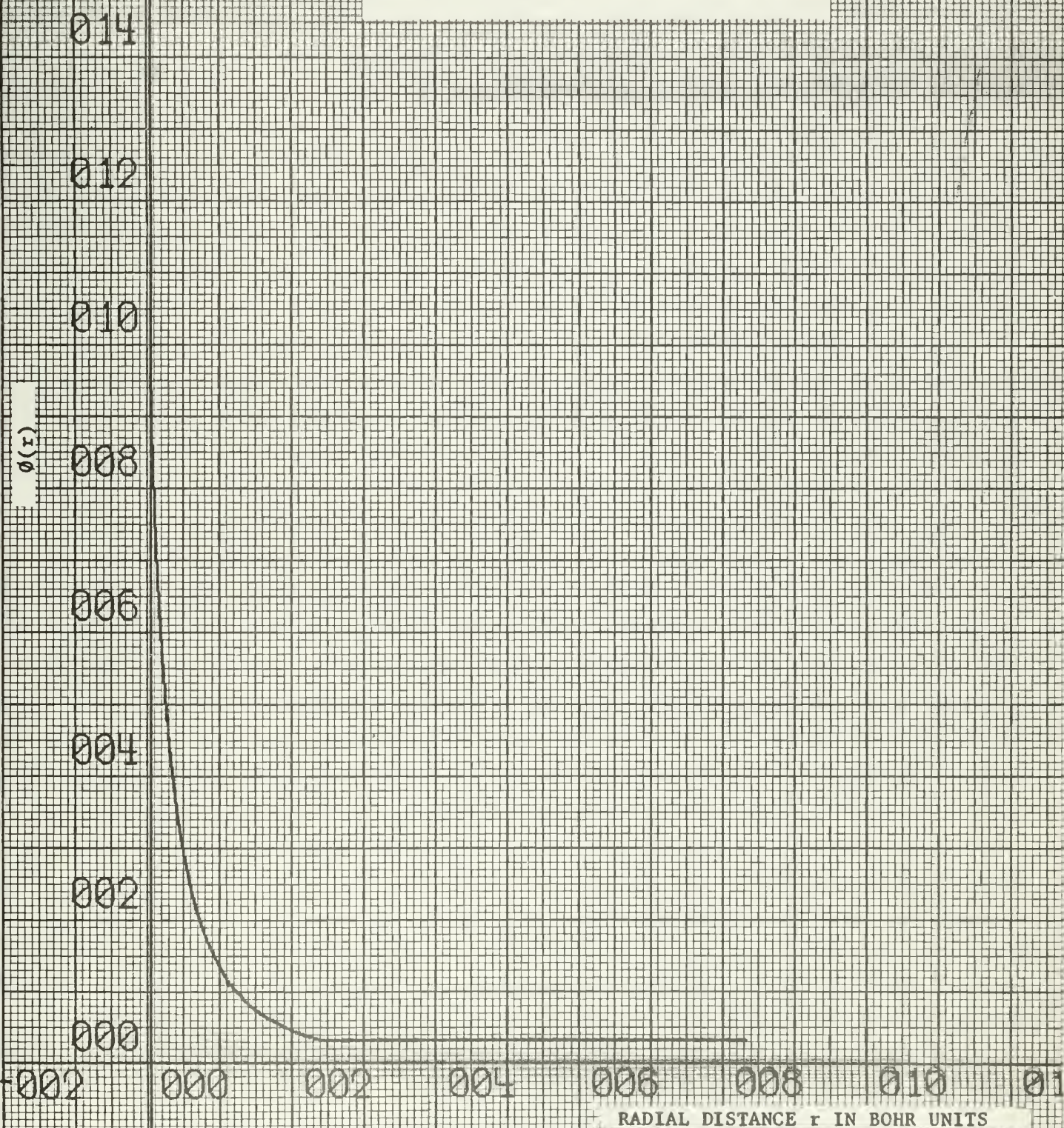


FIGURE 40

COPPER

RADIAL WAVE FUNCTION $R(r)$ vs.
RADIAL DISTANCE r

THOMAS-FERMI POTENTIAL

ENERGY STATE $E = .44$ RYDBERGS

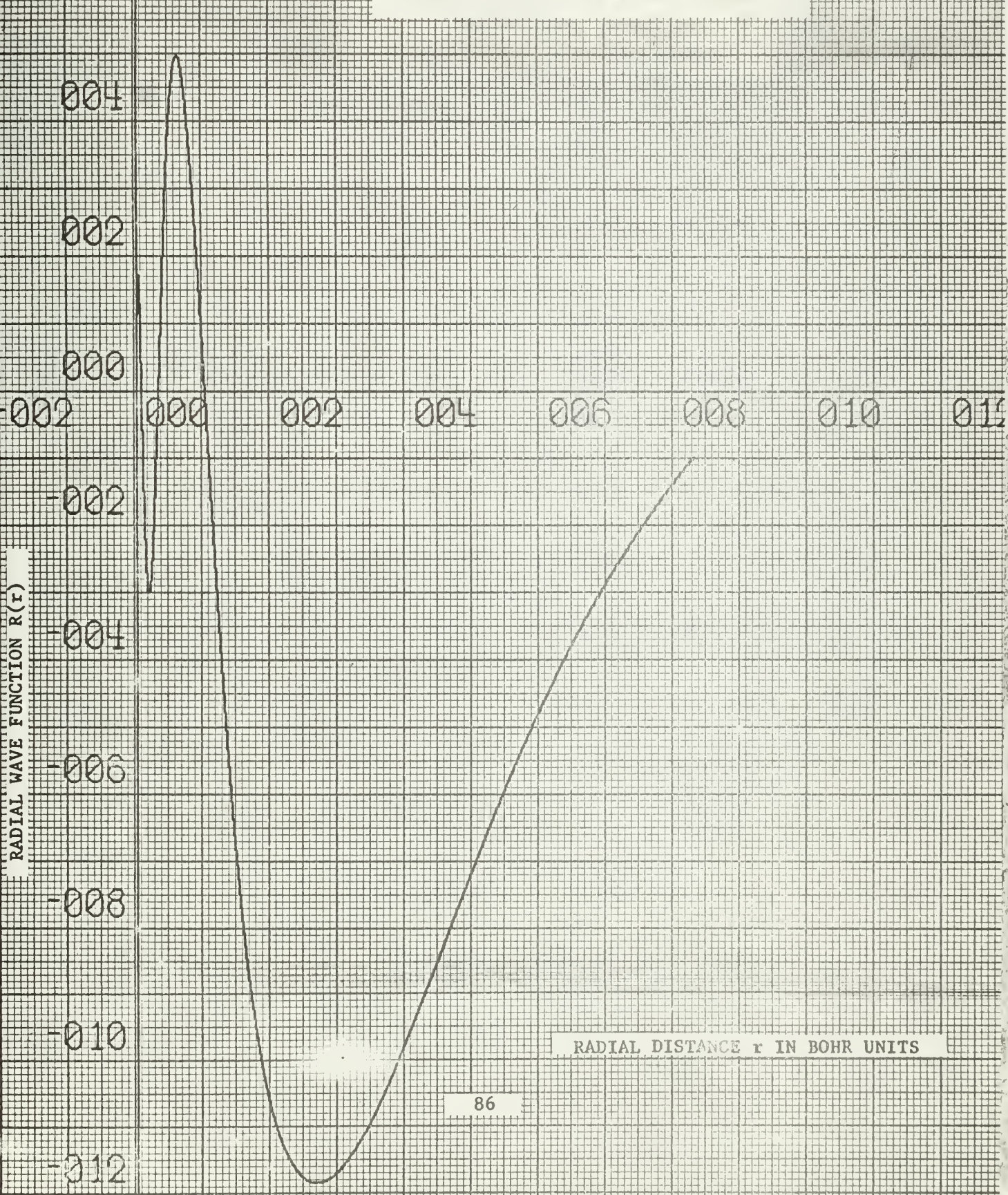


FIGURE 41
COPPER
RADIAL WAVE FUNCTION $R(r)$ vs.
RADIAL DISTANCE r
THOMAS-FERMI POTENTIAL
ENERGY STATE $E = .46$ RYDBERGS

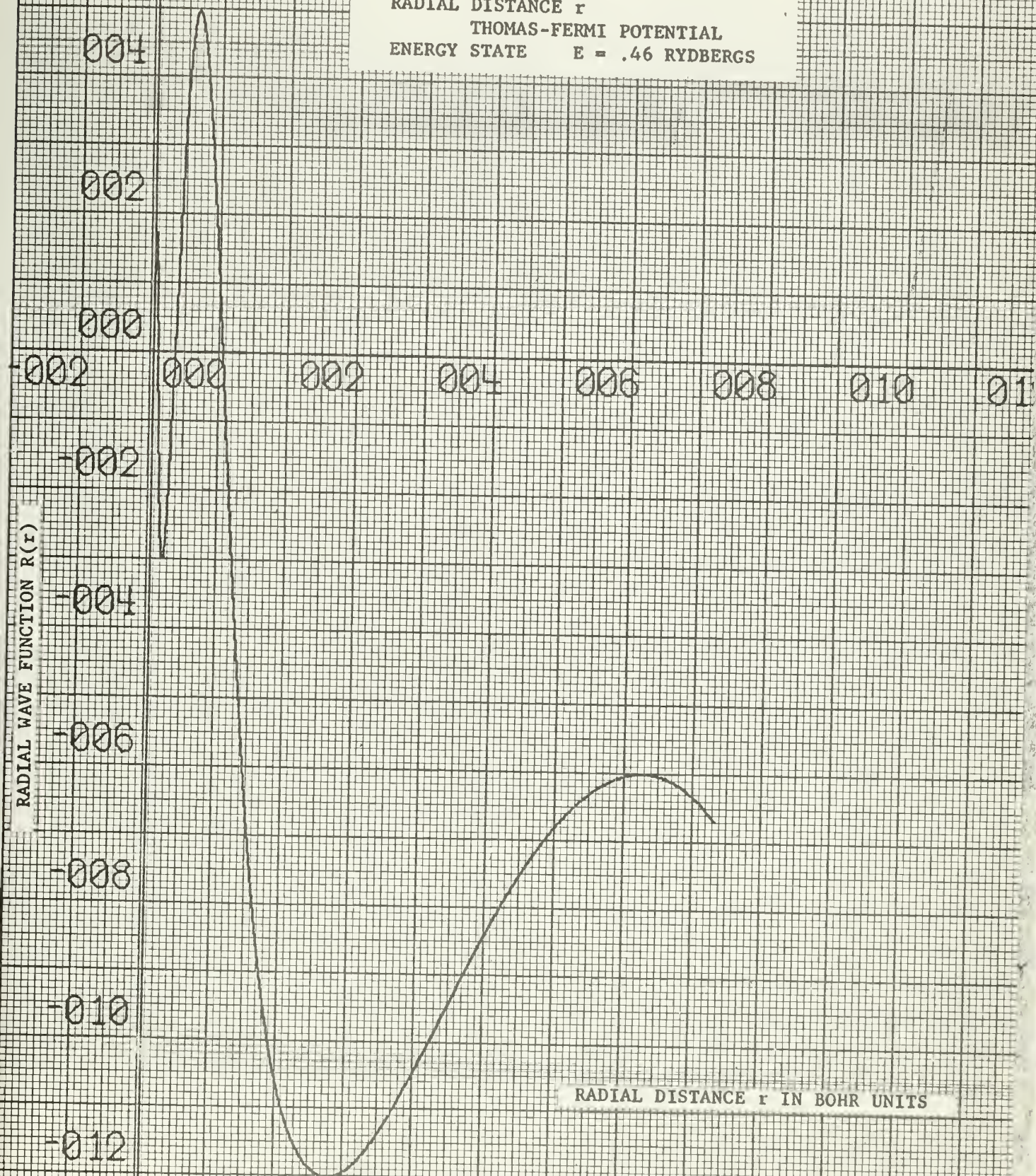


FIGURE 42
COPPER
RADIAL WAVE FUNCTION $R(r)$ vs.
RADIAL DISTANCE r
THOMAS-FERMI POTENTIAL
ENERGY STATE $E = .50$ RYDBERGS

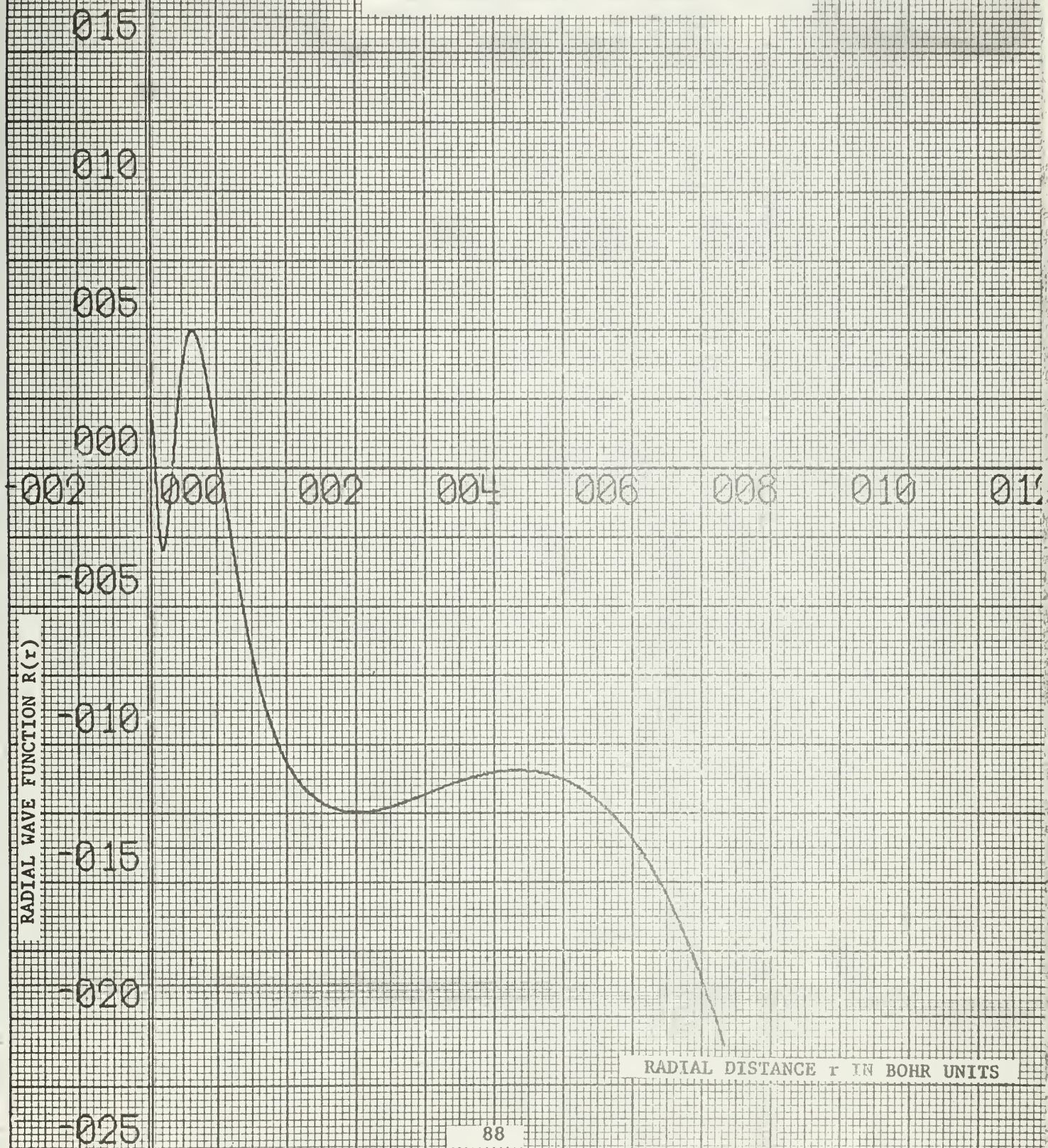


FIGURE 43

COPPER

RADIAL WAVE FUNCTION $R(r)$ vs.

RADIAL DISTANCE r

THOMAS-FERMI POTENTIAL

ENERGY STATE $E = .60$ RYDBERGS

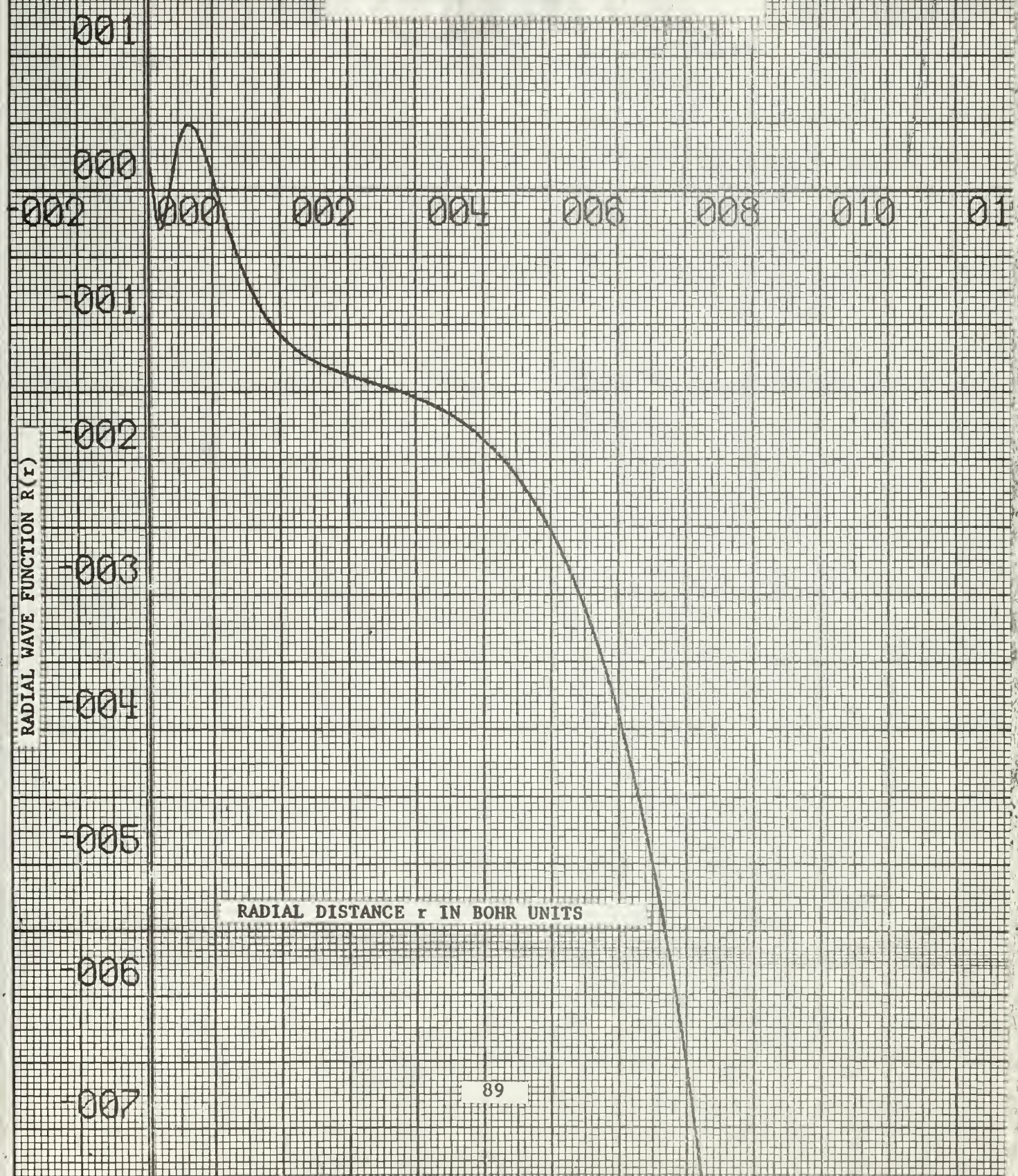


FIGURE 44
 COPPER
 RADIAL WAVE FUNCTION $R(r)$ vs.
 RADIAL DISTANCE r
 THOMAS-FERMI POTENTIAL
 ENERGY STATE $E = .80$ RYDBERGS

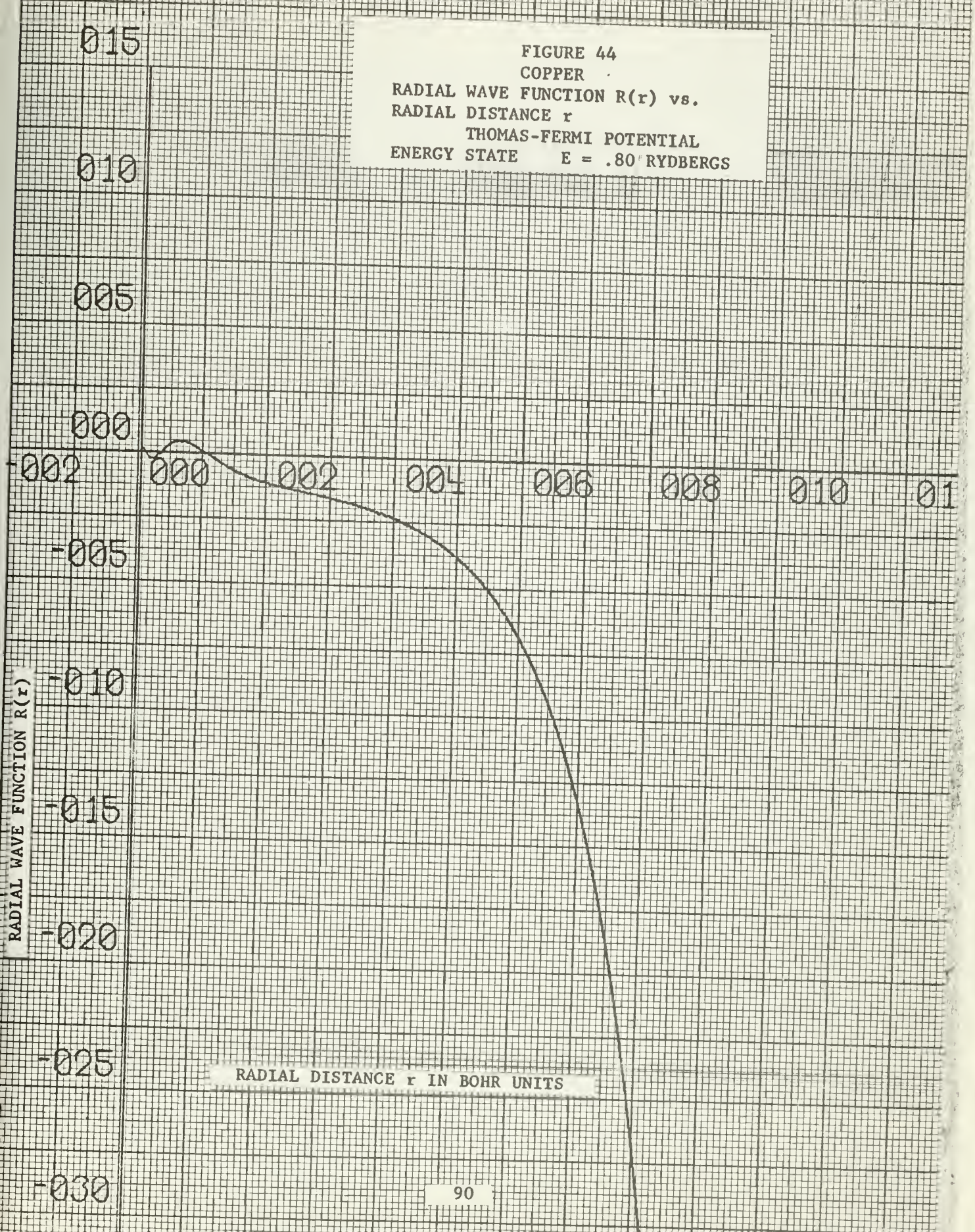


FIGURE 45.

COPPER

RADIAL WAVE FUNCTION $R(r)$ vs.

RADIAL DISTANCE r

THOMAS-FERMI POTENTIAL

ENERGY STATE $E = .87$ RYDBERGS

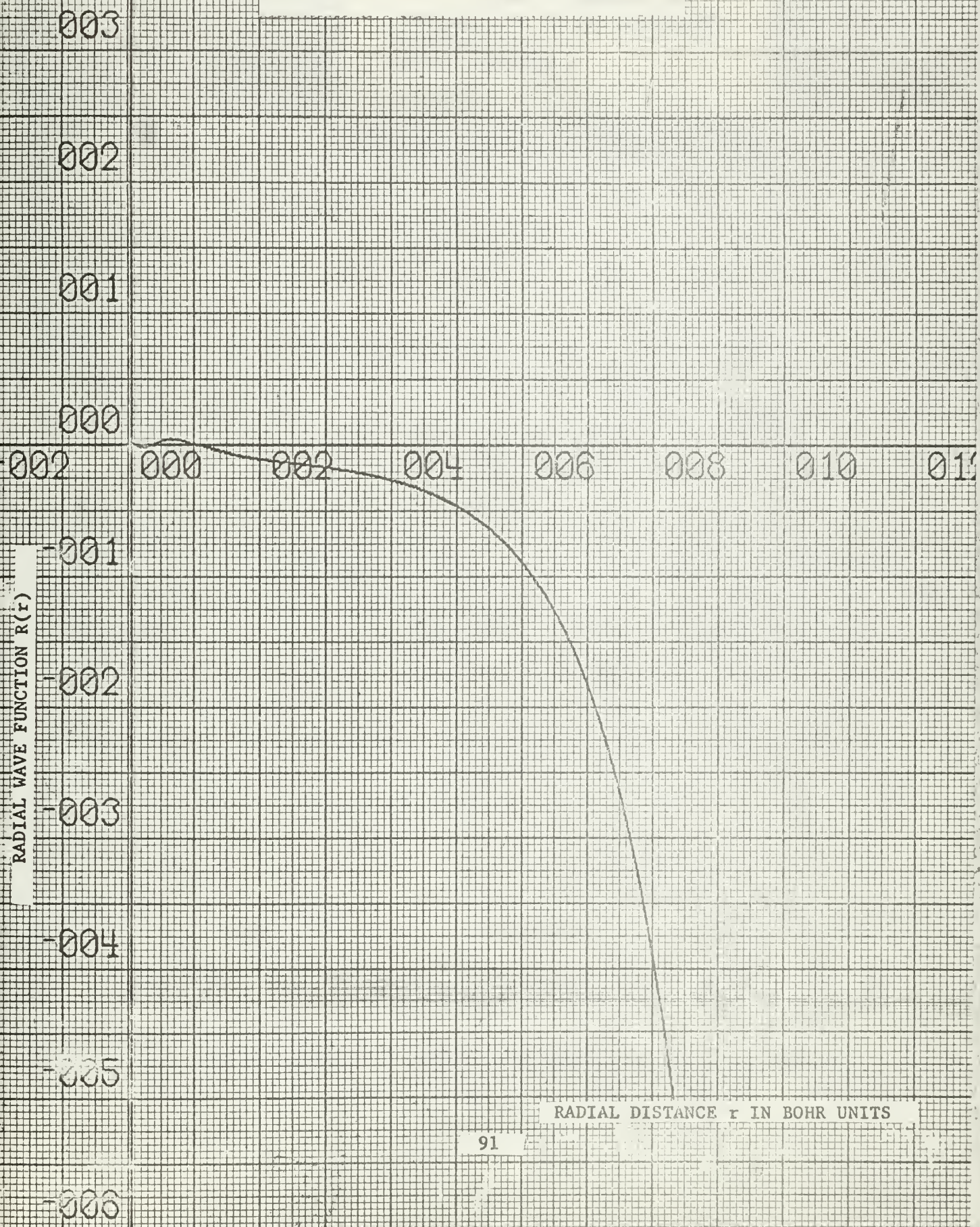


FIGURE 46
SILVER - THOMAS-FERMI
CONTRIBUTIONS TO THE EFFECTIVE
POTENTIAL $\phi(r)$ vs.
RADIAL DISTANCE r

$\phi(r)$

018
016
014
012
010
008
006
004
002
000
-002

000 002 004 006 008 010 012

RADIAL DISTANCE r IN BOHR UNITS

FIGURE 47
SILVER
THOMAS-FERMI POTENTIAL
ENERGY STATE $E = .28$ RYDBERGS

RADIAL WAVE FUNCTION $R(r)$

-002 000 002 004 006 008 010 01

RADIAL DISTANCE r IN BOHR UNITS

FIGURE 48
SILVER
THOMAS-FERMI POTENTIAL
ENERGY STATE $E = .30$ RYDBERGS

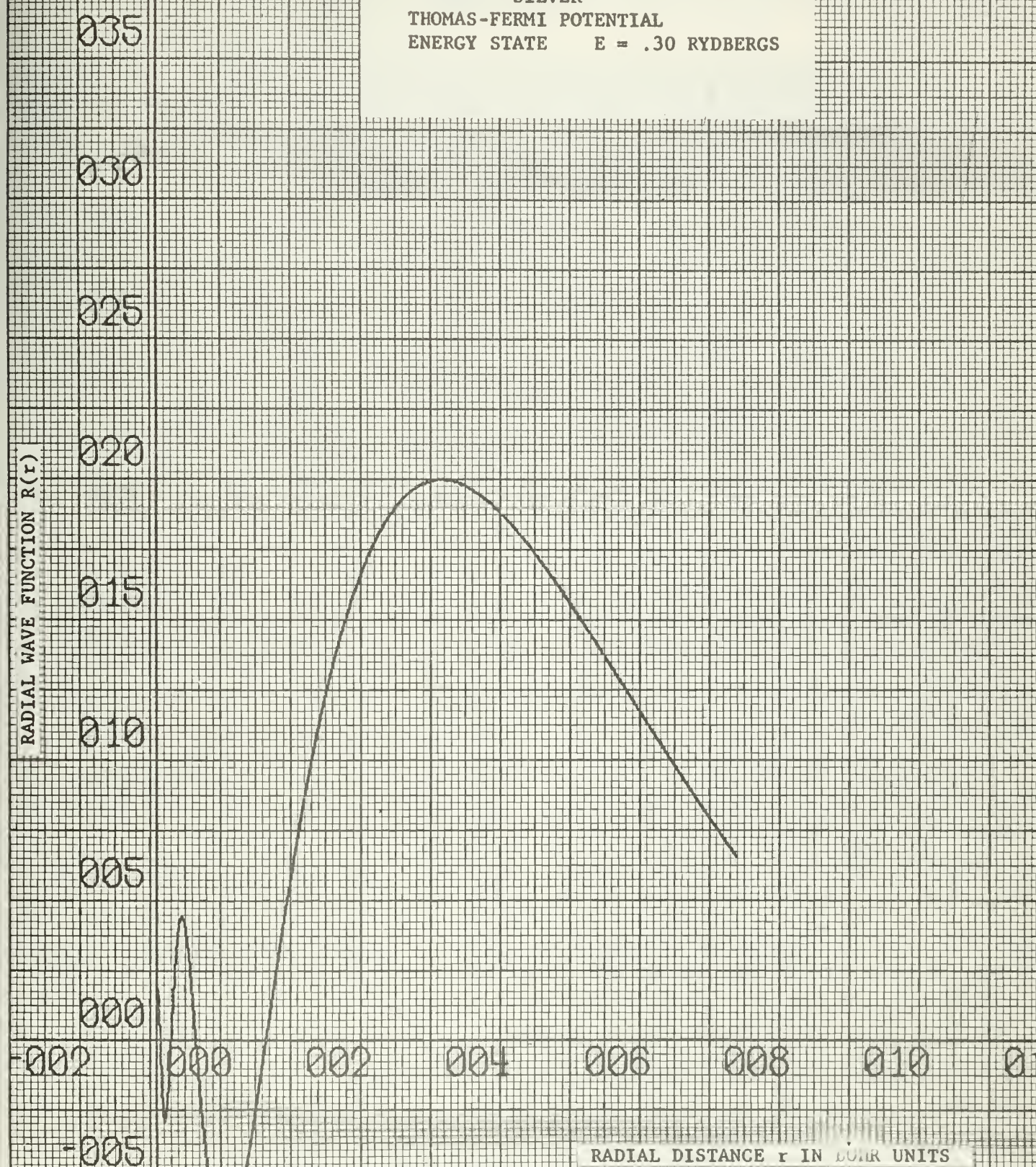
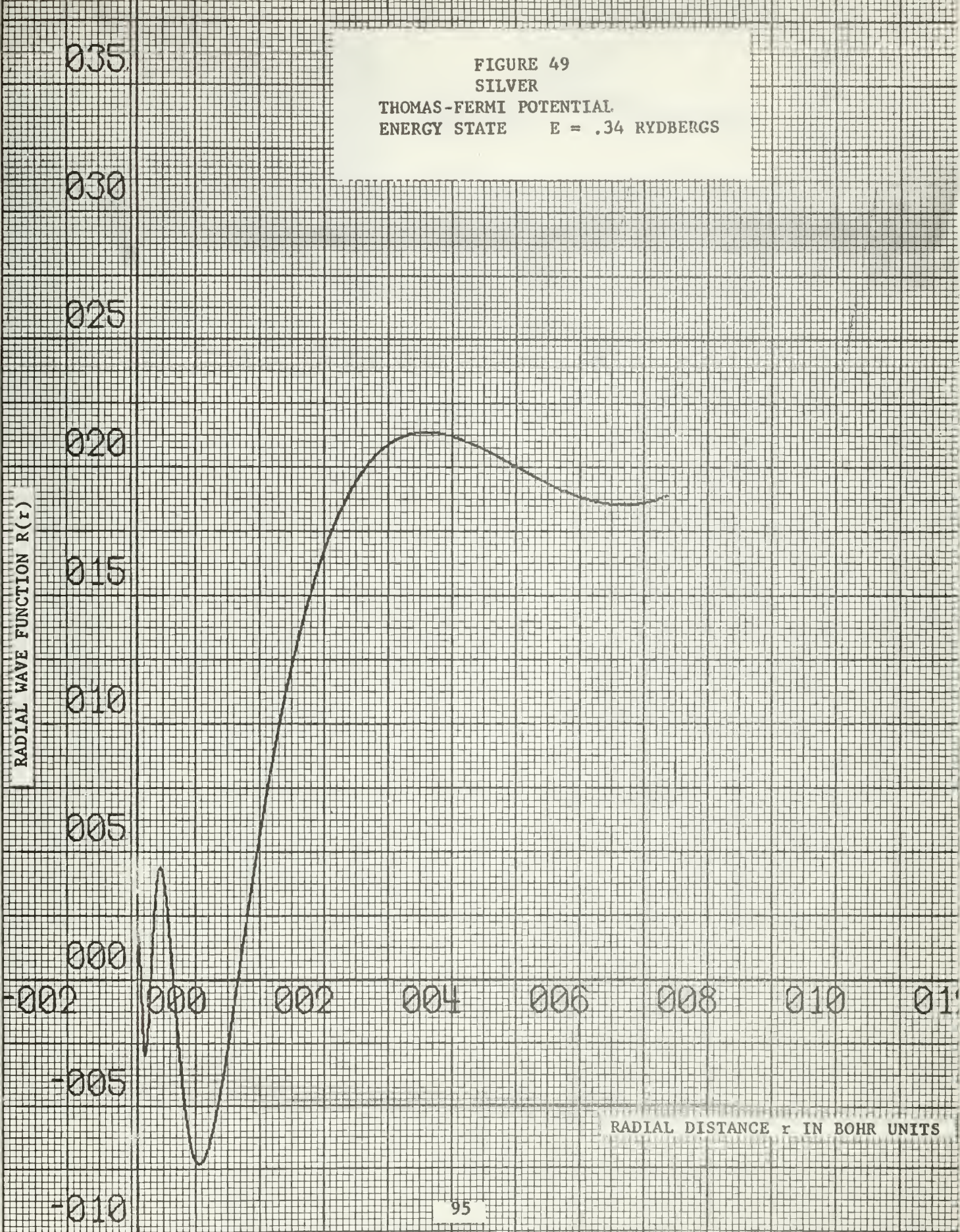


FIGURE 49
SILVER
THOMAS-FERMI POTENTIAL
ENERGY STATE $E = .34$ RYDBERGS

RADIAL WAVE FUNCTION $R(r)$



RADIAL DISTANCE r IN BOHR UNITS

FIGURE 50
SILVER
THOMAS-FERMI POTENTIAL
ENERGY STATE $E = .36$ RYDBERGS

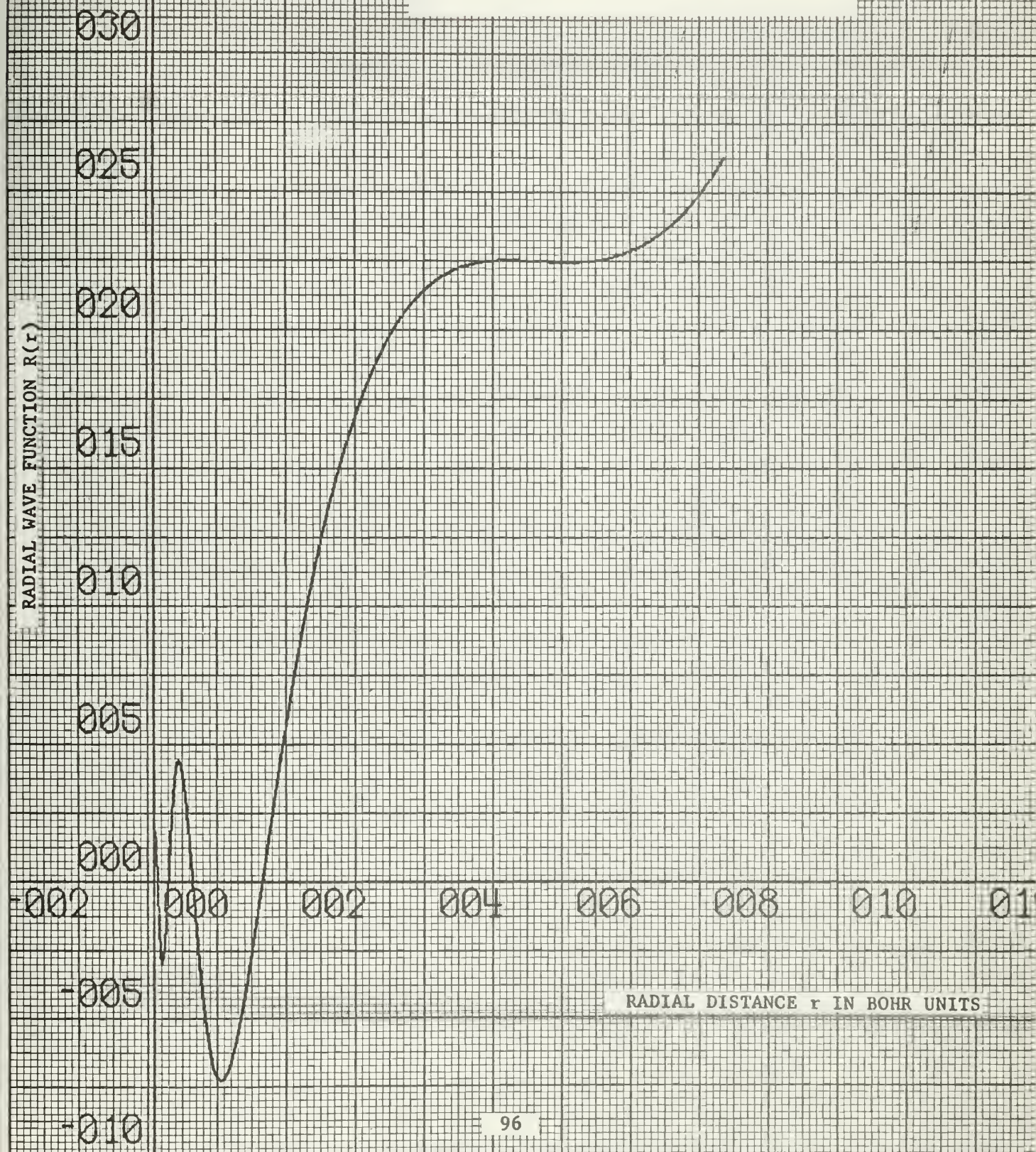
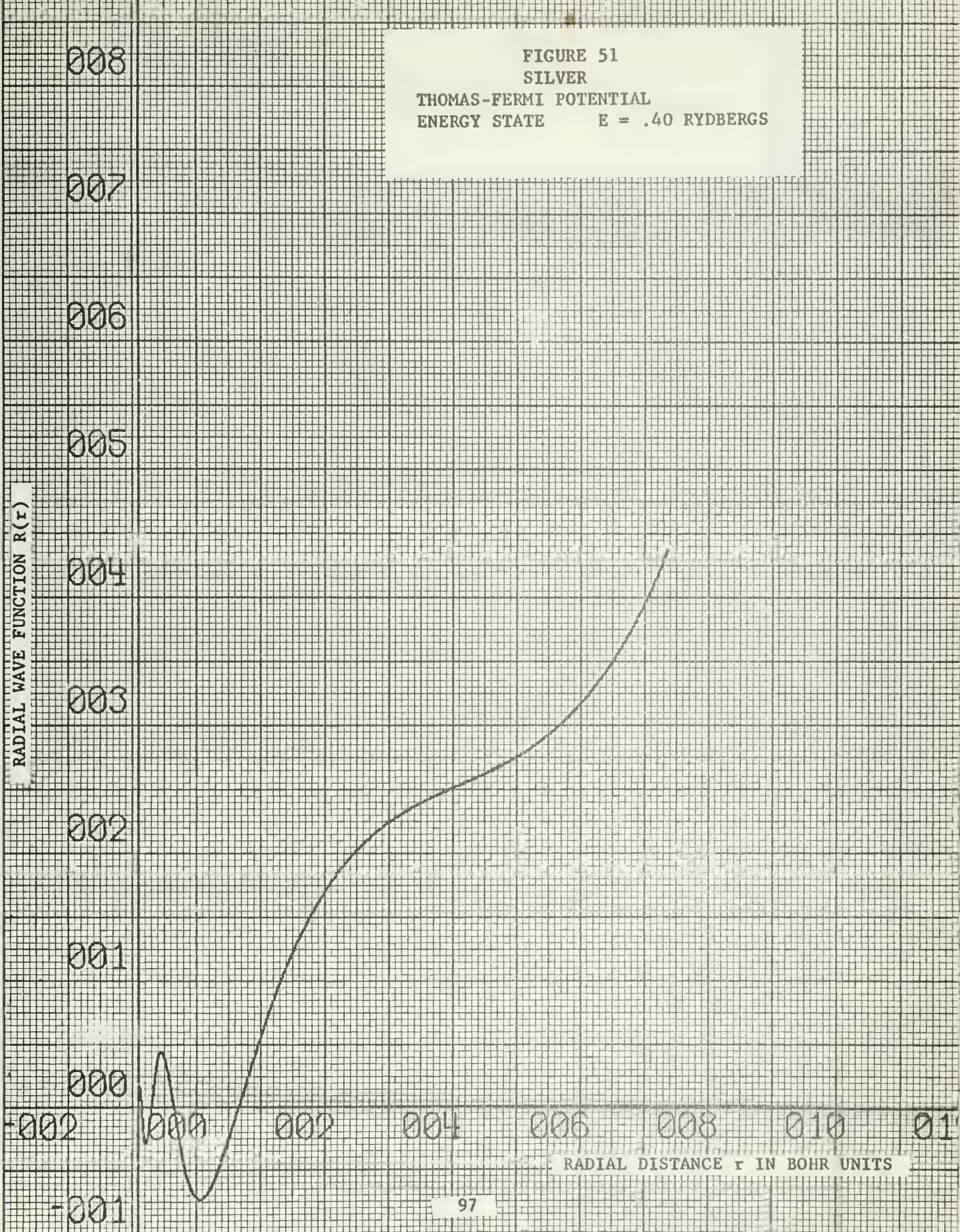


FIGURE 51
SILVER
THOMAS-FERMI POTENTIAL
ENERGY STATE $E = .40$ RYDBERGS

RADIAL WAVE FUNCTION $R(r)$



RADIAL DISTANCE r IN BOHR UNITS



17

18

19

20

21

22

23

24

25

26

FIGURE 52
SILVER
THOMAS-FERMI POTENTIAL
ENERGY STATE $E = .43$ RYDBERGS

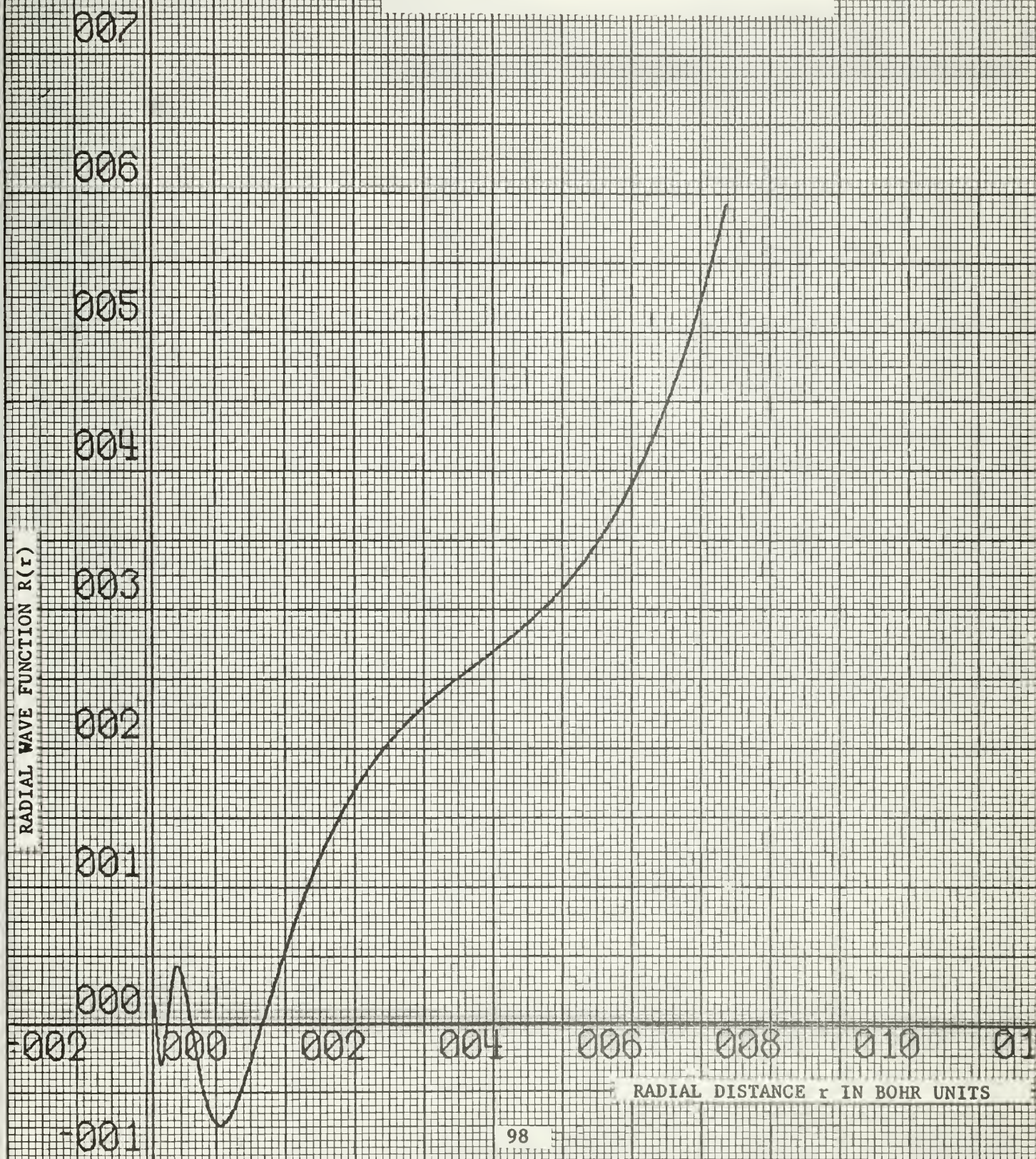


FIGURE 53

SILVER

THOMAS-FERMI POTENTIAL

ENERGY STATE $E = .50$ RYDBERGS

RADIAL WAVE FUNCTION $R(r)$

002 000 002 004 006 008 010 0

RADIAL DISTANCE r IN BOHR UNITS

FIGURE 54
SILVER - HARTREE
CONTRIBUTIONS TO THE EFFECTIVE
POTENTIAL $\phi(r)$ vs.
RADIAL DISTANCE $R(r)$

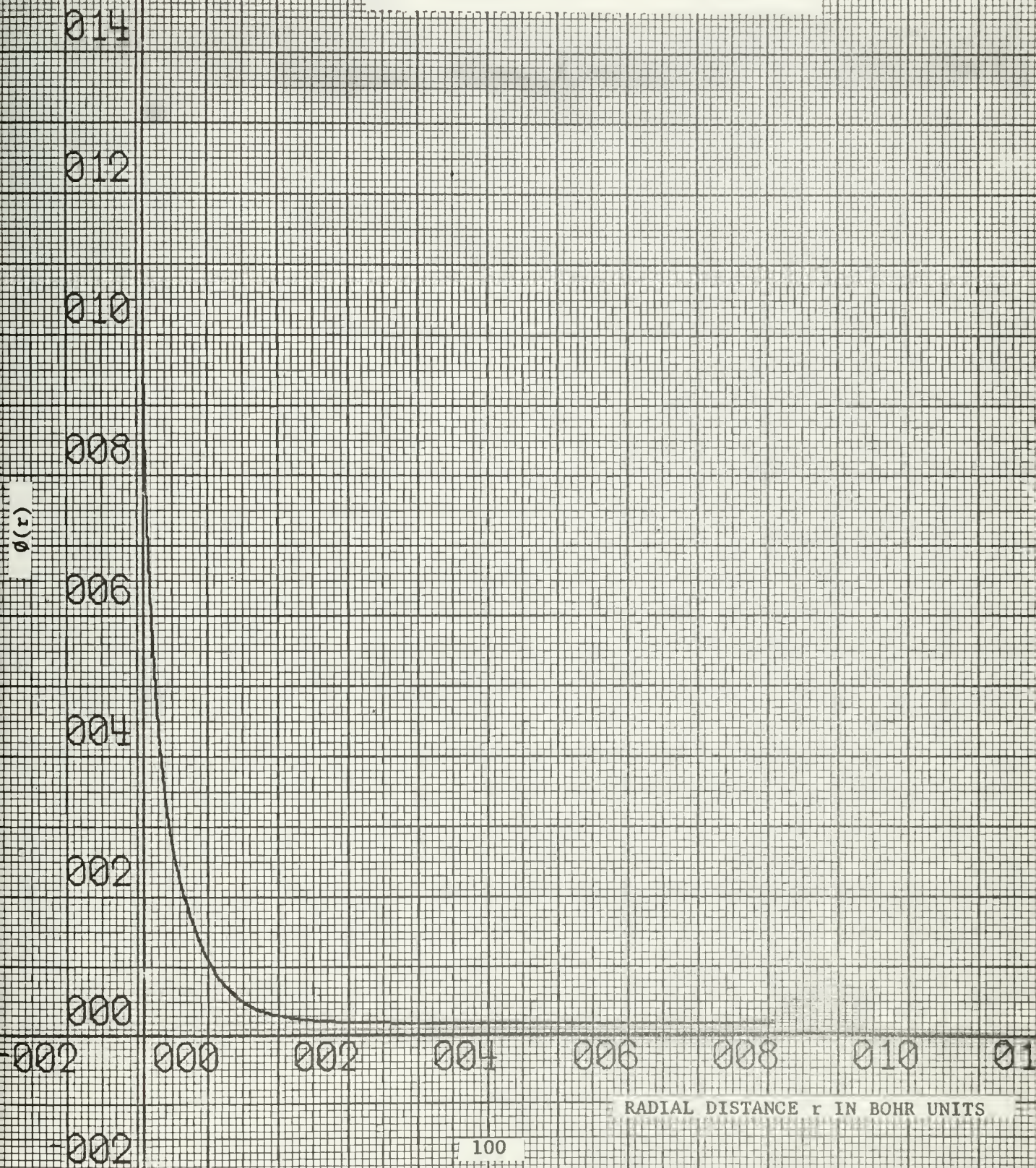


FIGURE 55
SILVER
RADIAL WAVE FUNCTION $R(r)$ vs.
RADIAL DISTANCE r
HARTREE POTENTIAL
ENERGY STATE $E = .28$ RYDBERGS

RADIAL WAVE FUNCTION $R(r)$

RADIAL DISTANCE r IN BOHR UNITS

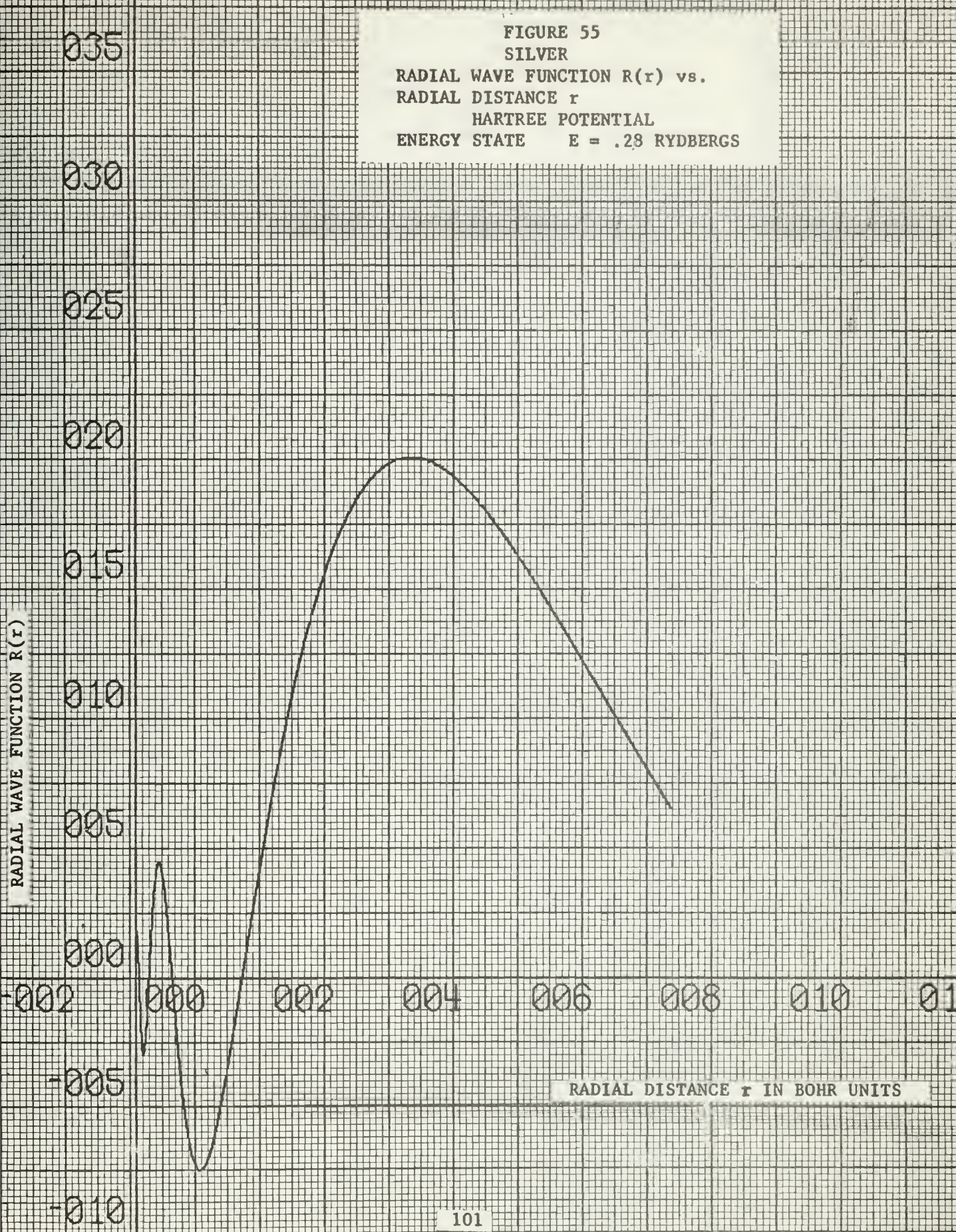
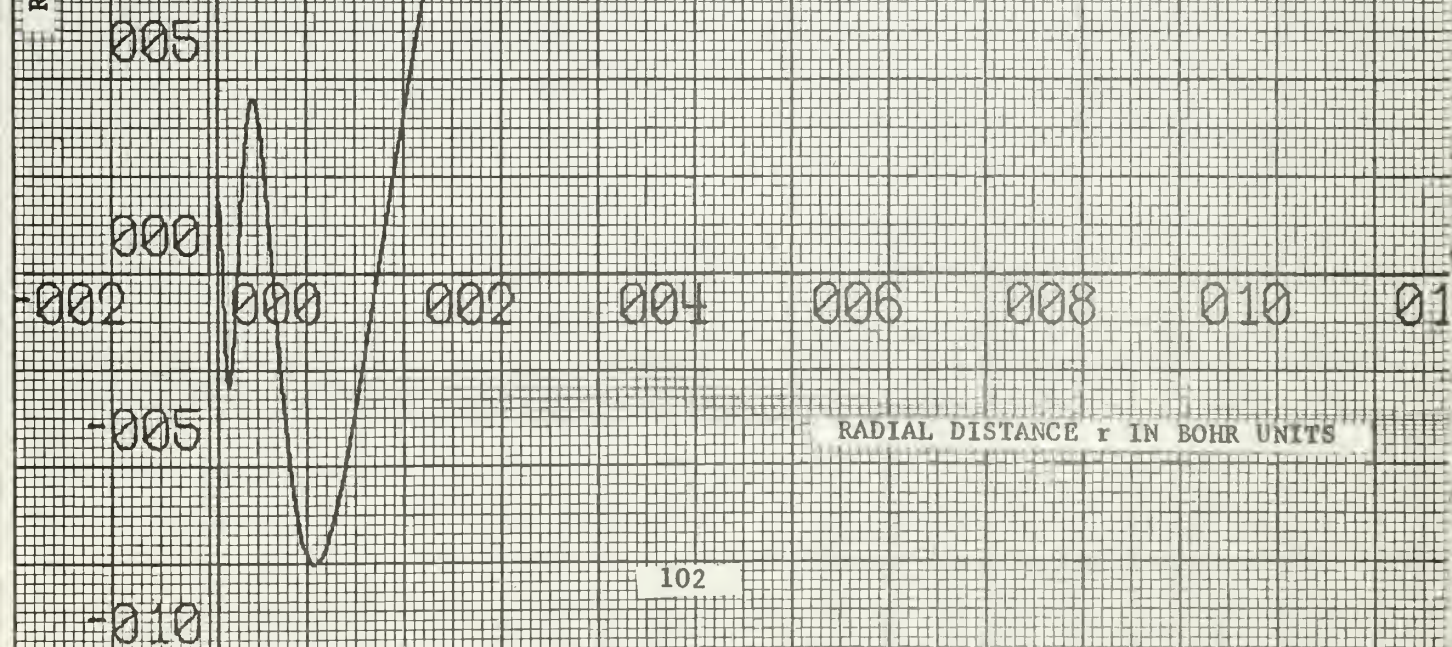


FIGURE 56
SILVER
RADIAL WAVE FUNCTION $R(r)$ vs.
RADIAL DISTANCE r
HARTREE POTENTIAL
ENERGY STATE $E = .30$ RYDBERGS

RADIAL WAVE FUNCTION $R(r)$



RADIAL DISTANCE r IN BOHR UNITS

FIGURE 57
SILVER
RADIAL WAVE FUNCTION $R(r)$ vs.
RADIAL DISTANCE r
HARTREE POTENTIAL
ENERGY STATE $E = .34$ RYDBERGS

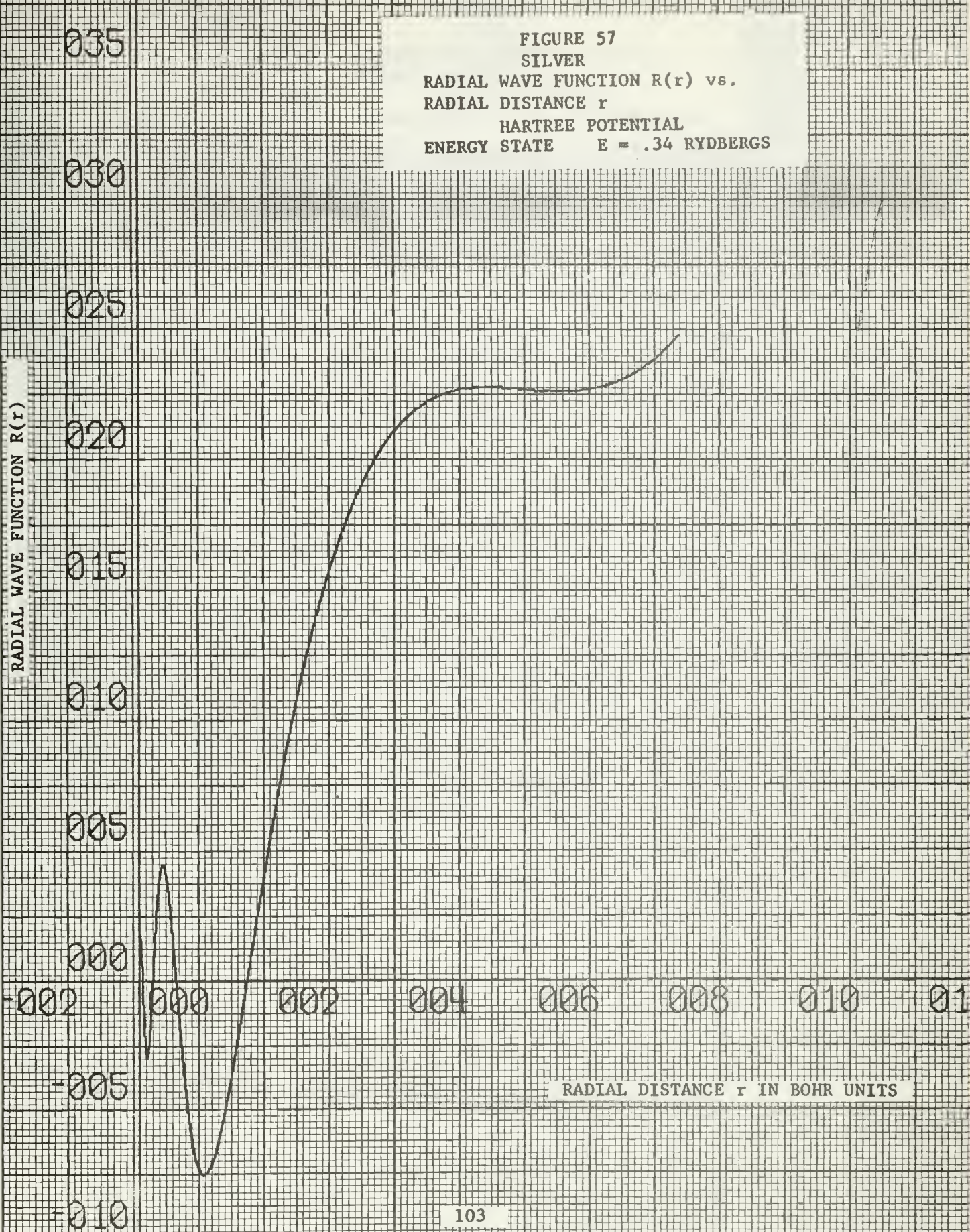


FIGURE 58

SILVER

RADIAL WAVE FUNCTION $R(r)$ vs.

RADIAL DISTANCE r

HARTREE POTENTIAL

ENERGY STATE $E = .36$ RYDBERGS

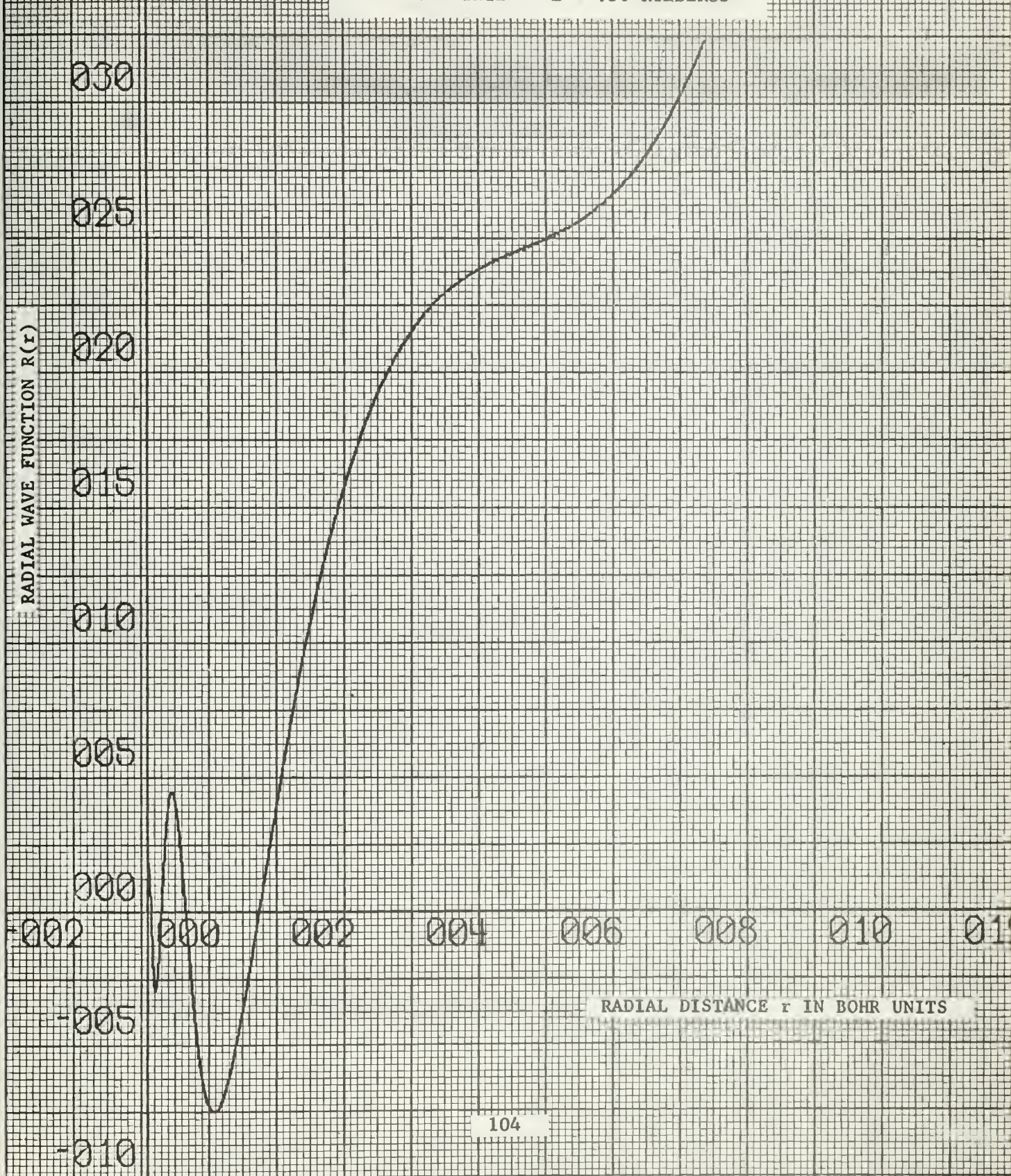
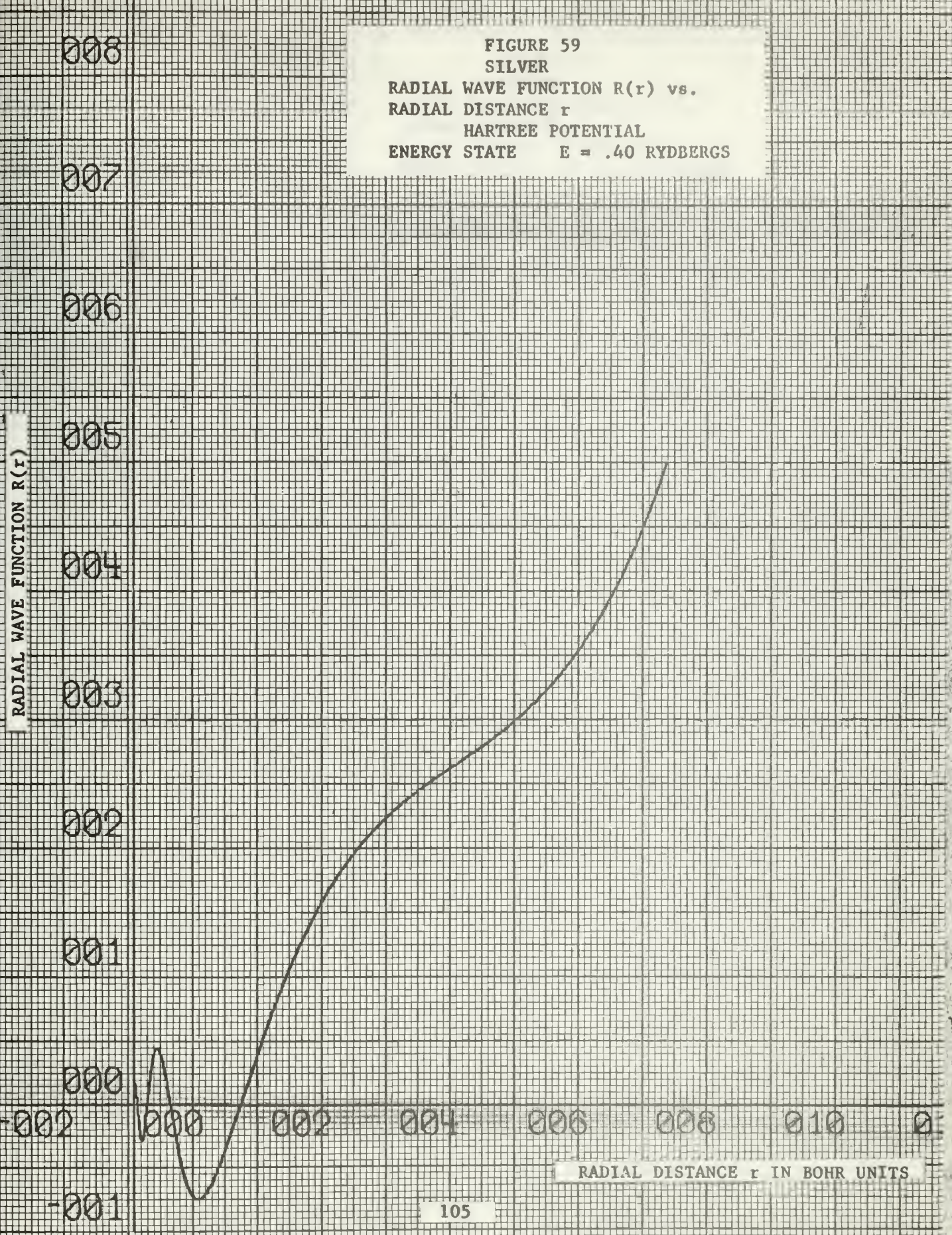


FIGURE 59
SILVER
RADIAL WAVE FUNCTION $R(r)$ vs.
RADIAL DISTANCE r
HARTREE POTENTIAL
ENERGY STATE $E = .40$ RYDBERGS

RADIAL WAVE FUNCTION $R(r)$



RADIAL DISTANCE r IN BOHR UNITS

FIGURE 60
SILVER
RADIAL WAVE FUNCTION $R(r)$ vs.
RADIAL DISTANCE r
HARTREE POTENTIAL
ENERGY STATE $E = .42$ RYDBERGS

RADIAL WAVE FUNCTION $R(r)$

-002 000 002 004 006 008 010 01

-001

RADIAL DISTANCE r IN BOHR UNITS

FIGURE 61
SILVER
RADIAL WAVE FUNCTION $R(r)$ vs.
RADIAL DISTANCE r
HARTREE POTENTIAL
ENERGY STATE $E = .43$ RYDBERGS

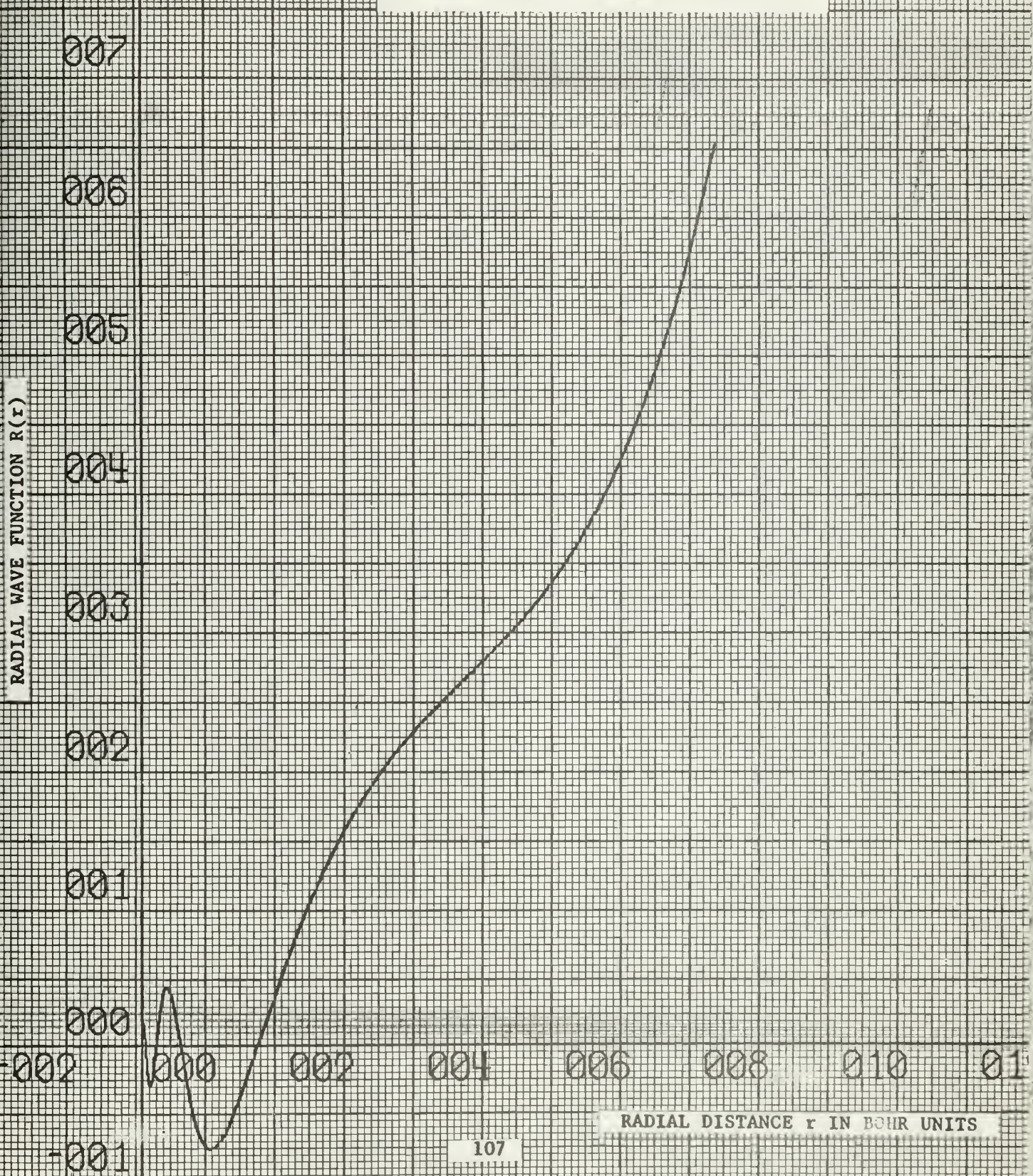


FIGURE 62
GOLD - THOMAS-FERMI
CONTRIBUTIONS TO THE EFFECTIVE
POTENTIAL $\phi(r)$ vs.
RADIAL DISTANCE r

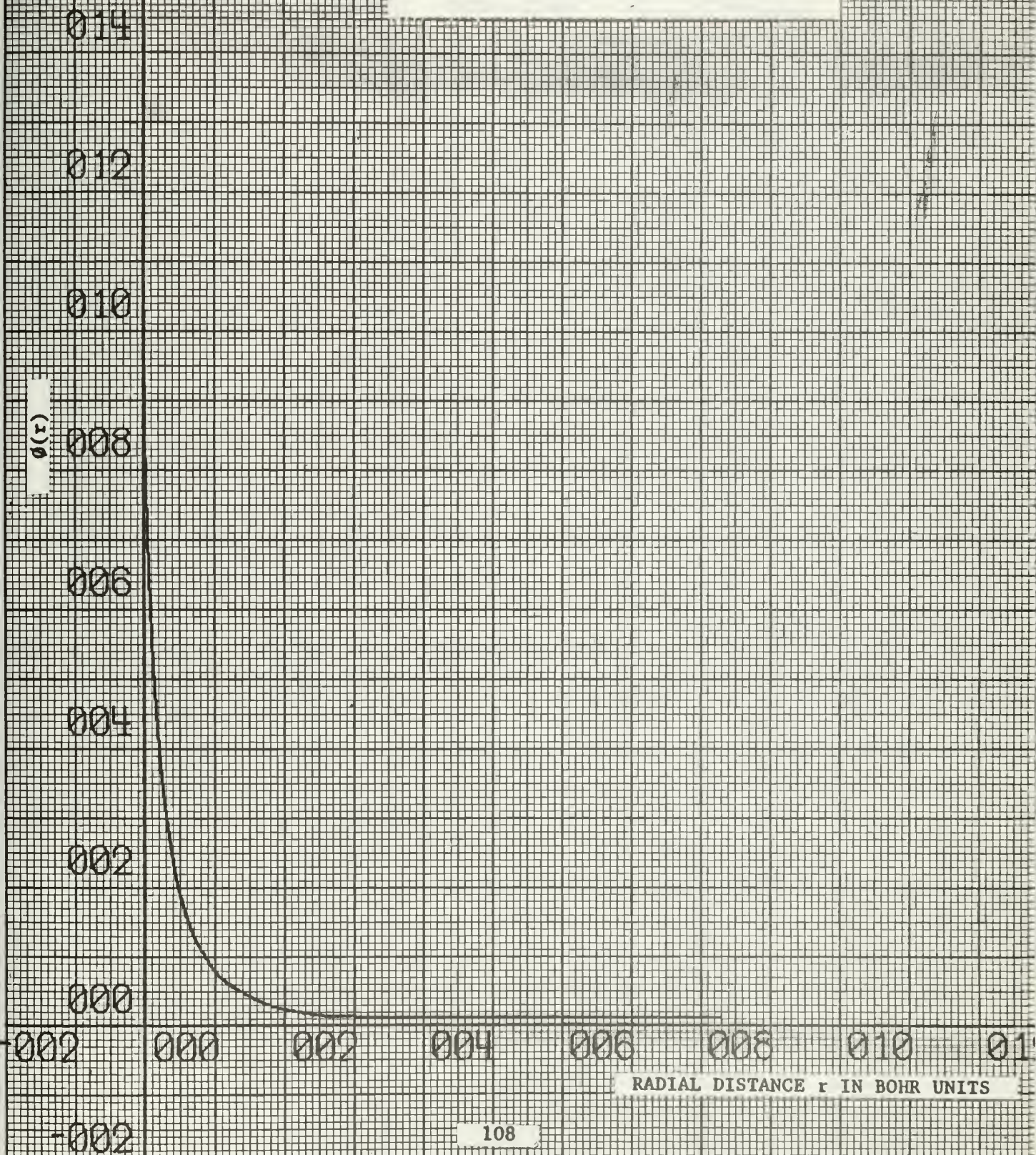


FIGURE 63

GOLD

RADIAL WAVE FUNCTION $R(r)$ vs.
RADIAL DISTANCE r

THOMAS-FERMI POTENTIAL

ENERGY STATE $E = .26$ RYDBERGS

RADIAL WAVE FUNCTION $R(r)$

005
004
003
002
001
000
-001
-002
-003
-004

RADIAL DISTANCE r IN BOHR UNITS

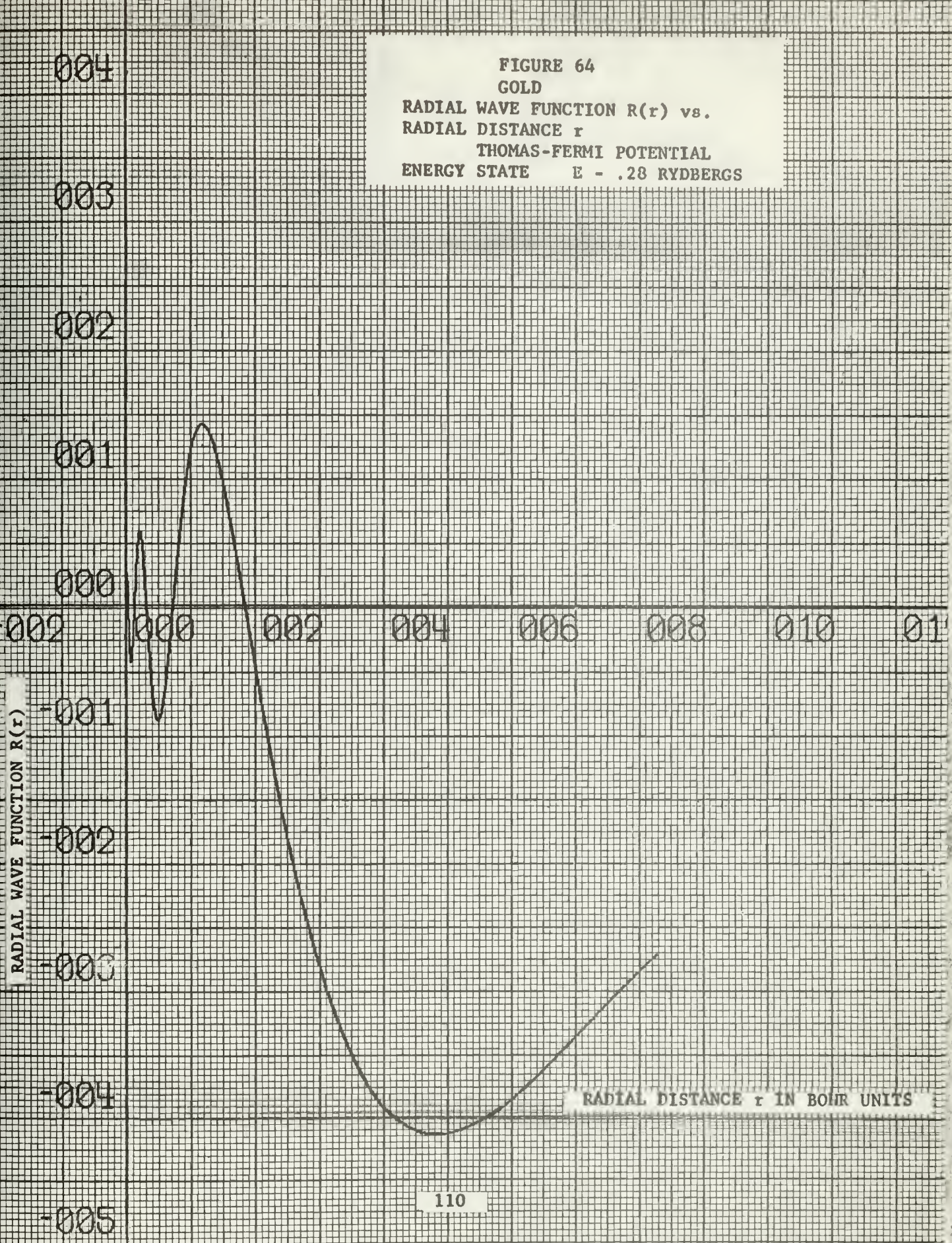


FIGURE 65

GOLD

RADIAL WAVE FUNCTION $R(r)$ vs.
RADIAL DISTANCE r

THOMAS-FERMI POTENTIAL

ENERGY STATE $E = .34$ RYDBERGS

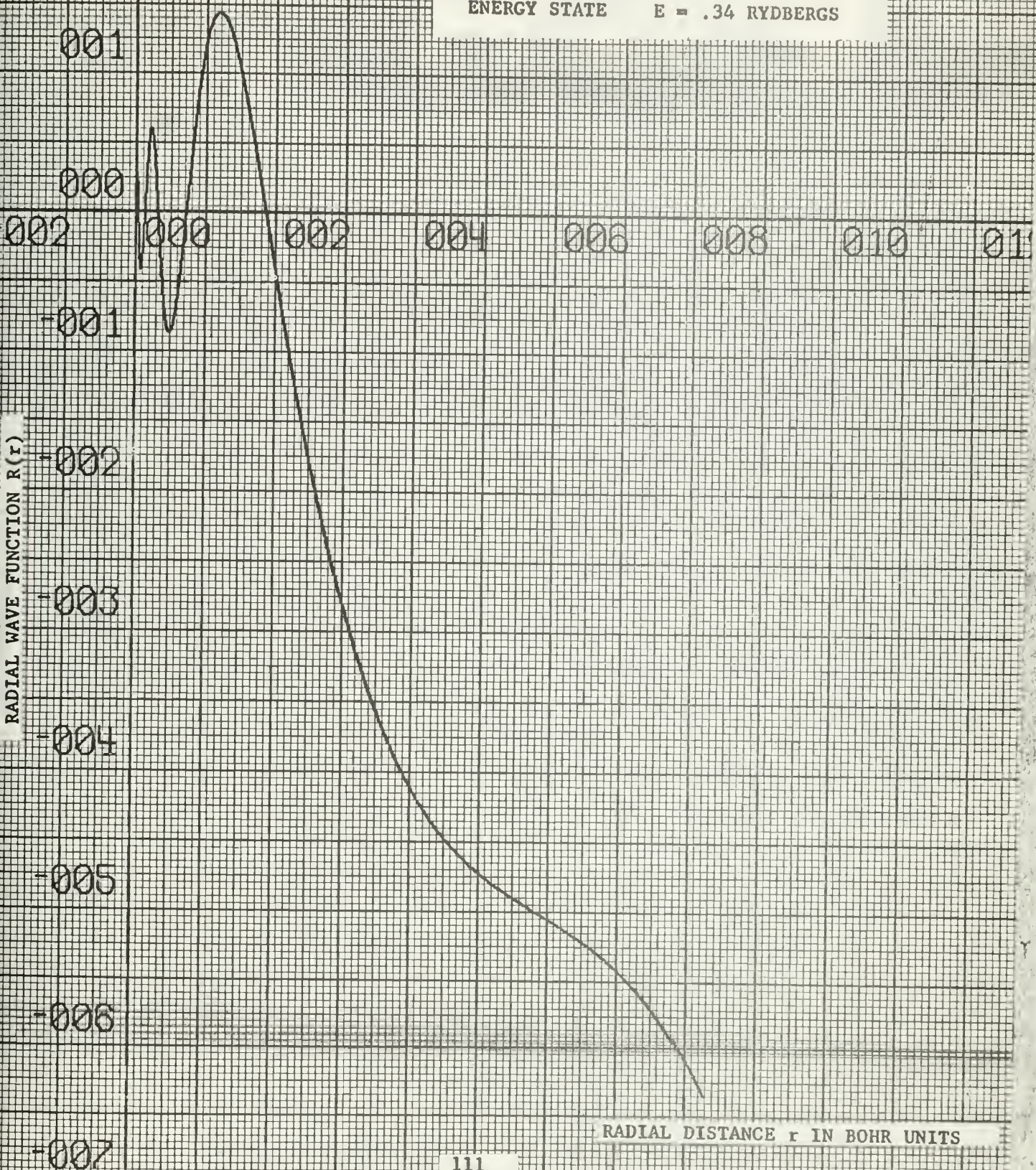
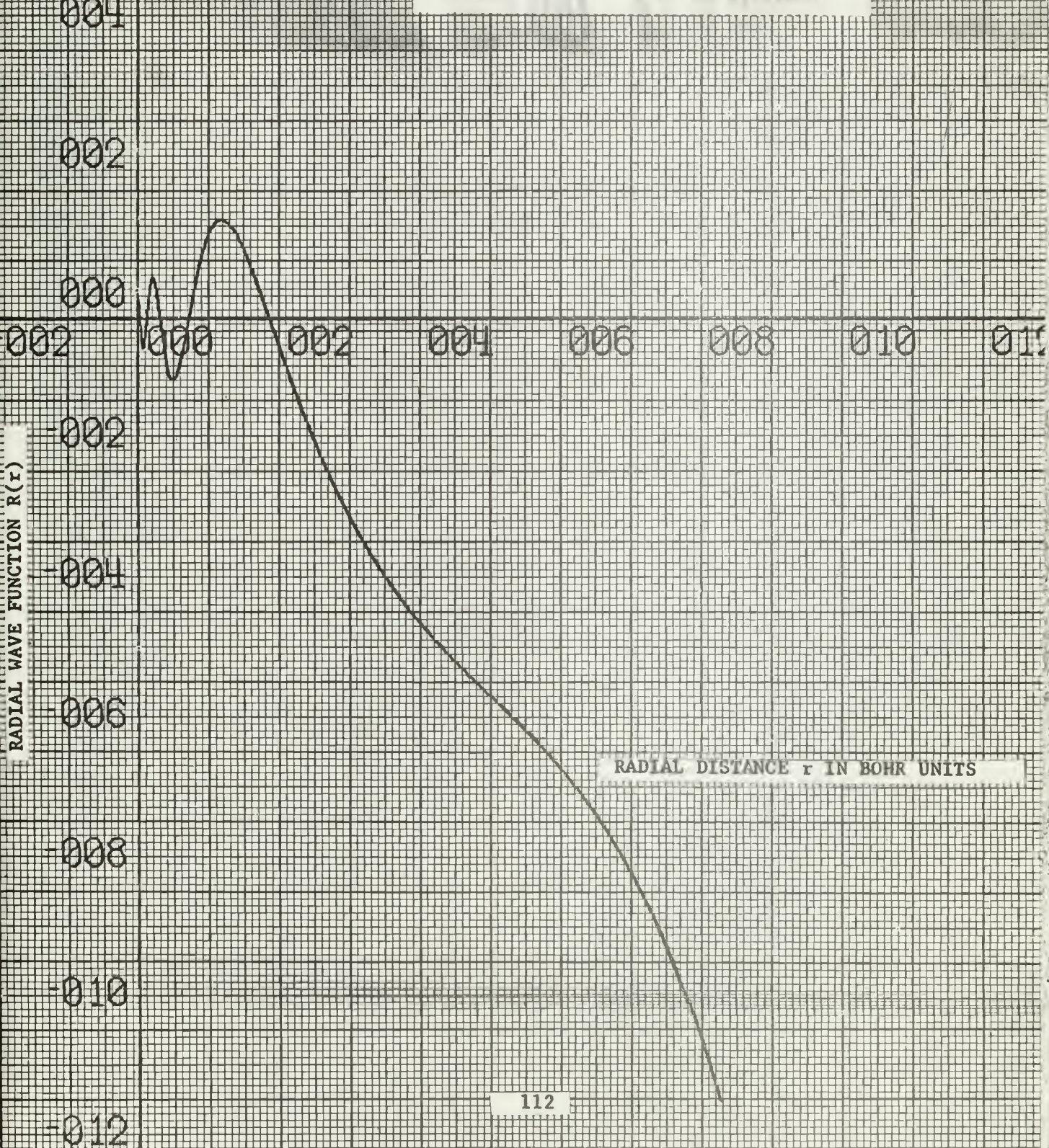


FIGURE 66
GOLD
RADIAL WAVE FUNCTION $R(r)$ vs.
RADIAL DISTANCE r
THOMAS-FERMI POTENTIAL
ENERGY STATE $E = .40$ RYDBERGS



004

FIGURE 67

GOLD

RADIAL WAVE FUNCTION $R(r)$ vs.RADIAL DISTANCE r

THOMAS-FERMI POTENTIAL

ENERGY STATE $E = .42$ RYDBERGS

002

000

-002

002

004

006

008

010

01

-002

-004

-006

-008

-010

-012

-014

RADIAL WAVE FUNCTION $R(r)$ RADIAL DISTANCE r IN BOHR UNITS

FIGURE 68
GOLD
RADIAL WAVE FUNCTION $R(r)$ vs.
RADIAL DISTANCE r
THOMAS-FERMI POTENTIAL
ENERGY STATE $E = .44$ RYDBERGS

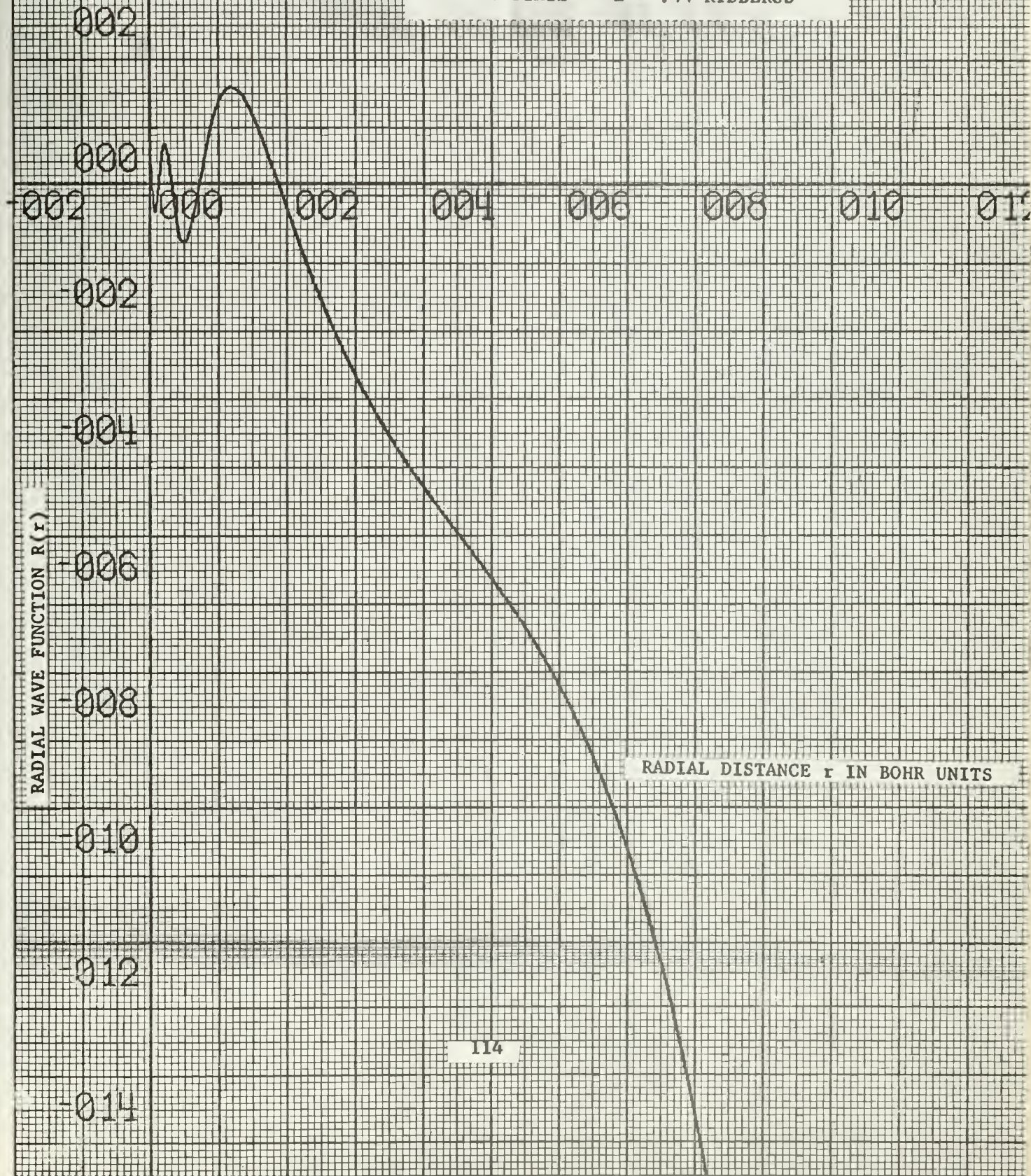


FIGURE 69
GOLD - HARTREE
CONTRIBUTIONS TO THE EFFECTIVE
POTENTIAL $\phi(r)$ vs.
RADIAL DISTANCE r

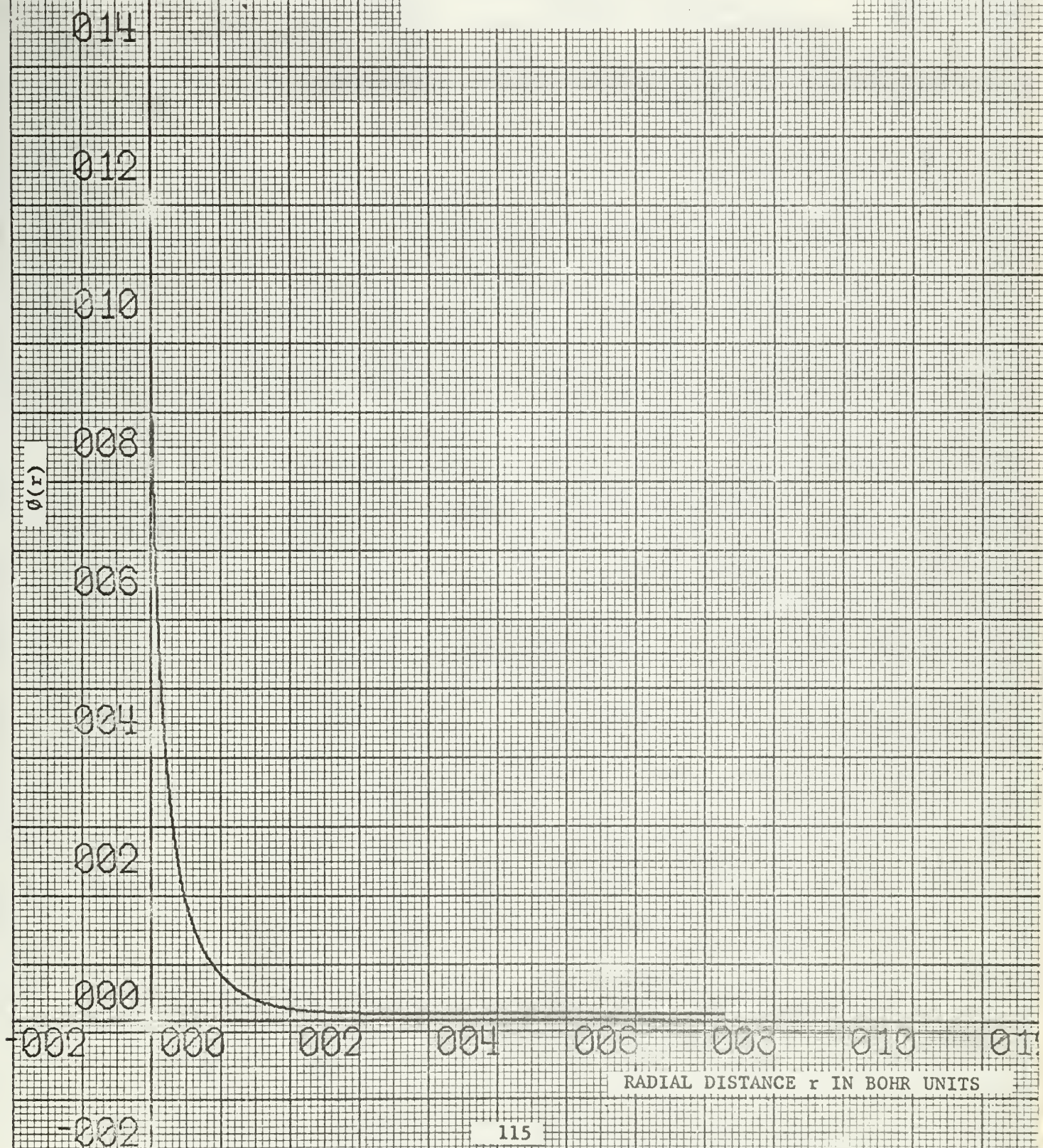


FIGURE 70
GOLD
RADIAL WAVE FUNCTION $R(r)$ vs.
RADIAL DISTANCE r
HARTREE POTENTIAL
ENERGY STATE $E = .26$ RYDBERGS

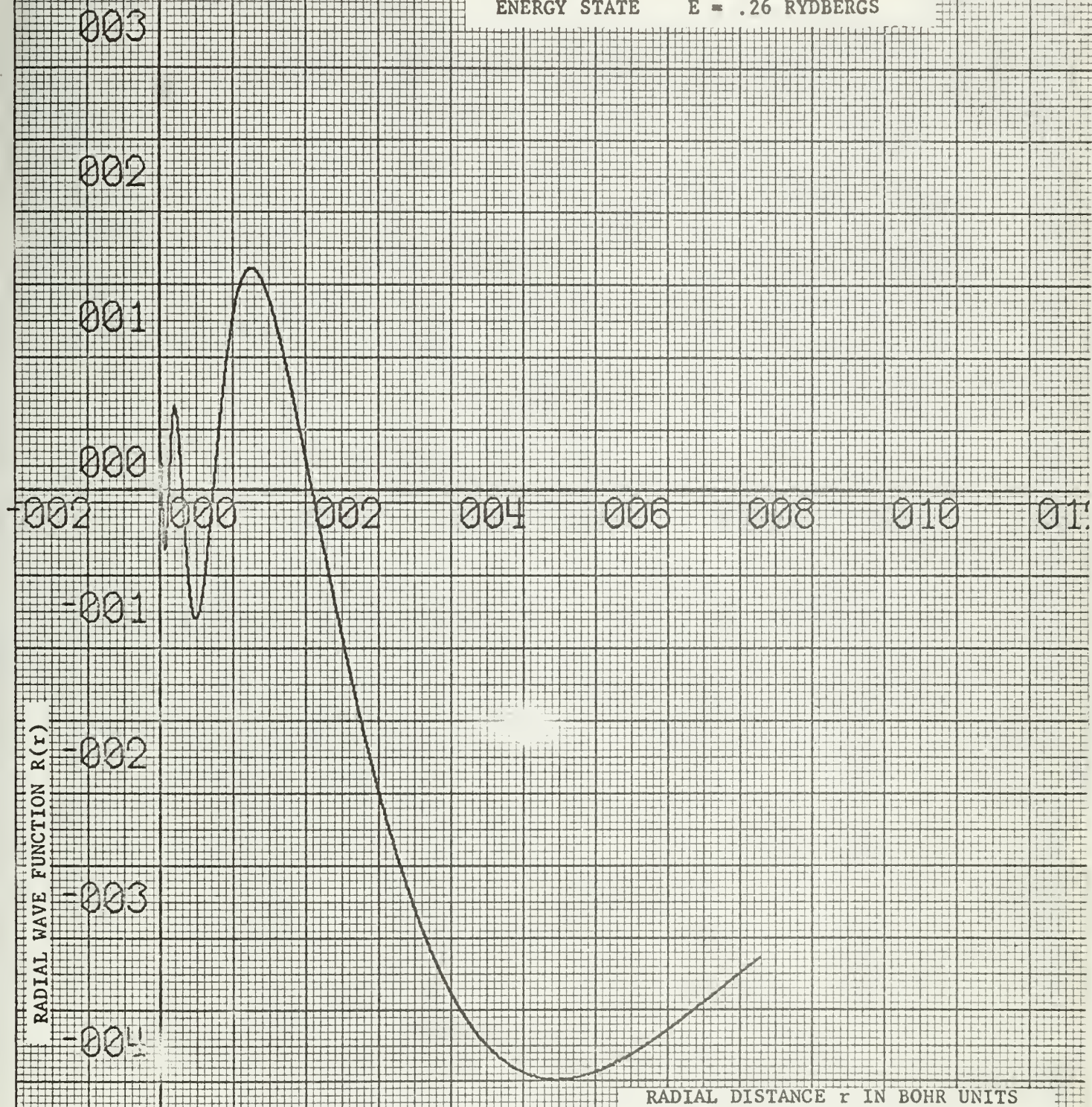


FIGURE 71

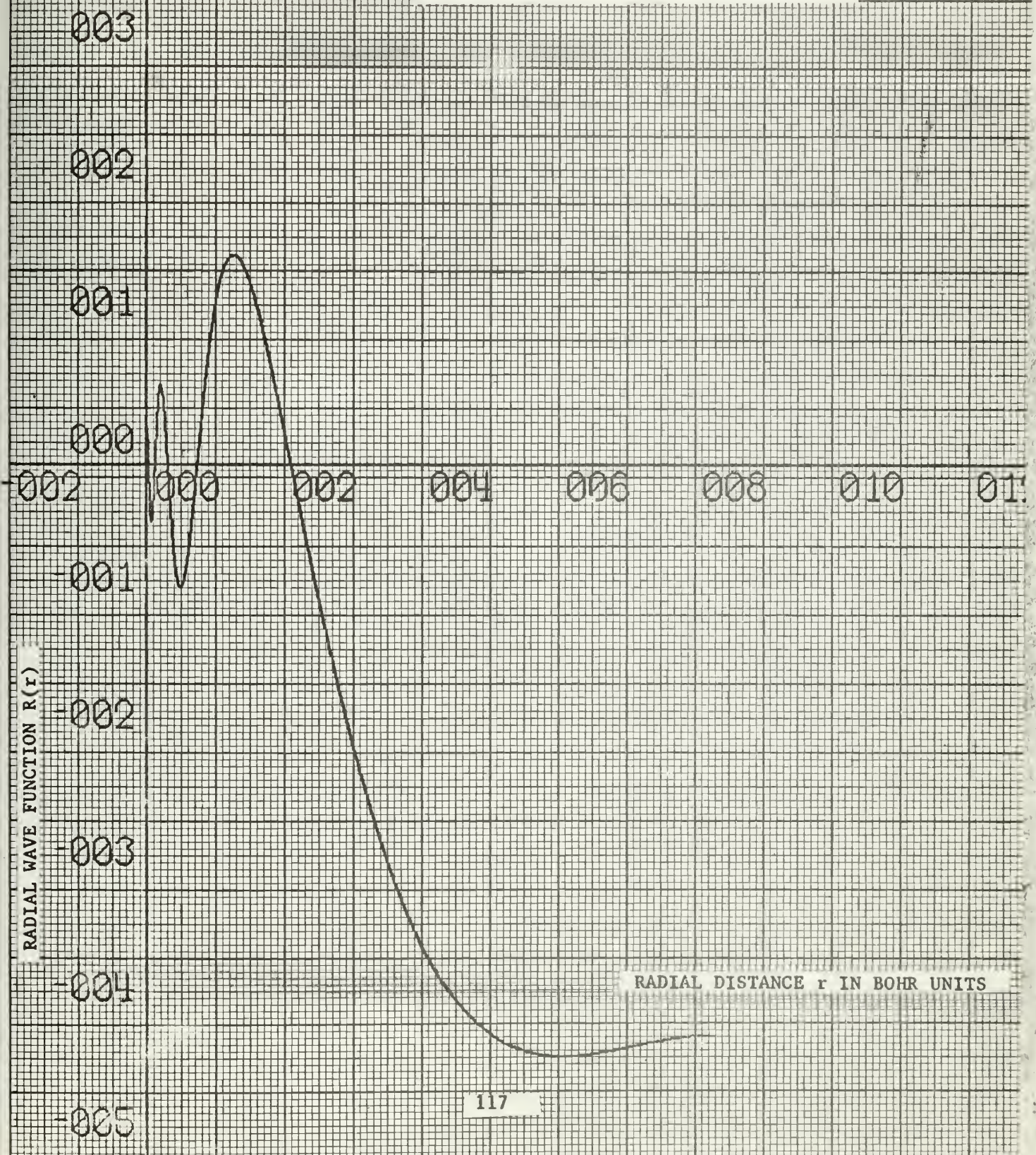
GOLD

RADIAL WAVE FUNCTION $R(r)$ vs.

RADIAL DISTANCE r

HARTREE POTENTIAL

ENERGY STATE $E = .28$ RYDBERGS



010

FIGURE 72

GOLD

RADIAL WAVE FUNCTION $R(r)$ vs.RADIAL DISTANCE r

HARTREE POTENTIAL

ENERGY STATE $E = .34$ RYDBERGS

008

006

004

002

000

-002

000

002

004

006

008

010

012

RADIAL WAVE FUNCTION $R(r)$

-002

-004

-006

-008

RADIAL DISTANCE r IN BOHR UNITS

006

FIGURE 73

GOLD

RADIAL WAVE FUNCTION $R(r)$ vs.RADIAL DISTANCE r

HARTREE POTENTIAL

ENERGY STATE $E = .40$ RYDBERGS

004

002

000

-002 000 002 004 006 008 010 01

-002

-004

-006

-008

-010

-012

RADIAL WAVE FUNCTION $R(r)$ RADIAL DISTANCE r IN BOHR UNITS

004

FIGURE 74

GOLD

RADIAL WAVE FUNCTION $R(r)$ vs.RADIAL DISTANCE r

HARTREE POTENTIAL

ENERGY STATE $E = .42$ RYDBERGS

002

000

-002

000

002

004

006

008

010

012

-002

-004

-006

-008

-010

-012

-014

RADIAL WAVE FUNCTION $R(r)$ RADIAL DISTANCE r IN BOHR UNITS

004

002

000

-002

-004

-006

-008

-010

-012

-014

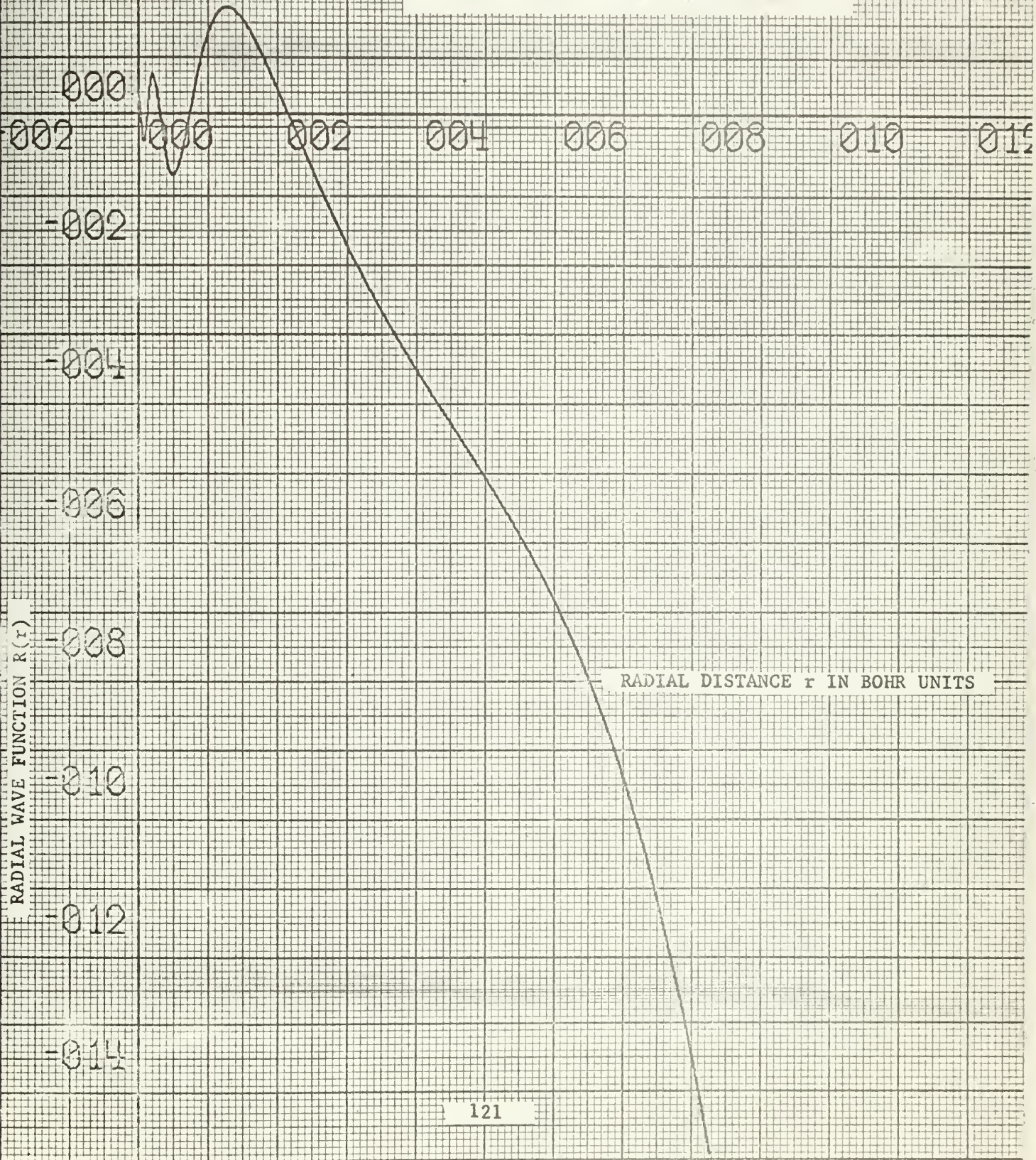
-016

FIGURE 75

GOLD

RADIAL WAVE FUNCTION $R(r)$ vs.
RADIAL DISTANCE r

HARTREE POTENTIAL

ENERGY STATE $E = .44$ RYDBERGSRADIAL DISTANCE r IN BOHR UNITS

APPENDIX III

TABULATED VALUES OF THE WAVE FUNCTIONS OF GOLD

TABLE V

GOLF

PHI(R) CONTRIBUTIONS TO THE EFFECTIVE POTENTIAL
AND THE RADIAL WAVE FUNCTION. IONIZATION
ENERGY=.656 RYDBERGS. R IS IN UNITS OF 1/100
BOHR UNITS.

R	PHI(R)	R(R)
1	9.201099244E-01	7.63658744E-03
2	8.46086760E-01	2.80568509E-02
3	5.13447670E-01	2.97255569E-02
4	7.86723391E-01	1.86613450E-02
5	7.63776204E-01	1.70924405E-03
6	7.43550420E-01	-1.54969909E-02
7	7.25250004E-01	-2.27601009E-02
8	7.08587379E-01	-3.91534965E-02
9	6.93217200E-01	-4.30701115E-02
10	6.78922012E-01	-4.17480428E-02
11	6.65539202E-01	-3.50504547E-02
12	6.52040977E-01	-2.67195355E-02
13	6.41026945E-01	-1.51914269E-02
14	6.29715610E-01	-2.40175468E-02
15	6.18939770E-01	1.04041254E-02
16	6.08643420E-01	2.24124015E-02
17	5.98772544E-01	3.34630022E-02
18	5.89230772E-01	4.24537750E-02
19	5.80193422E-01	4.92751134E-02
20	5.71406617E-01	5.36755603E-02
21	5.62921003E-01	5.54990711E-02
22	5.54713919E-01	5.53391223E-02
23	5.46764399E-01	5.27911068E-02
24	5.39054790E-01	4.92520297E-02
25	5.31563592E-01	4.20138007E-02
26	5.24291507E-01	3.43665924E-02
27	5.17210366E-01	2.56273373E-02
28	5.10313339E-01	1.61139900E-02
29	5.03582663E-01	6.13744216E-03
30	4.97029527E-01	-4.00698048E-03
31	4.90622417E-01	-1.40467797E-02
32	4.84336522E-01	-2.37362406E-02
33	4.78224524E-01	-3.28596569E-02
34	4.72235732E-01	-4.10232827E-02
35	4.66399070E-01	-4.93703946E-02
36	4.60652504E-01	-5.51526774E-02
37	4.55024426E-01	-6.04901310E-02
38	4.49505492E-01	-6.46562433E-02
39	4.44091074E-01	-6.76192337E-02
40	4.38776722E-01	-6.93681019E-02
41	4.33559350E-01	-6.99204976E-02
42	4.28433253E-01	-6.94092377E-02
43	4.23391909E-01	-6.78955217E-02
44	4.18440637E-01	-6.48142586E-02
45	4.13570440E-01	-6.10746109E-02
46	4.08791342E-01	-5.64513671E-02
47	4.04066557E-01	-5.10396606E-02
48	3.99425446E-01	-4.49378554E-02
49	3.94835538E-01	-3.82482111E-02
50	3.90354479E-01	-3.10741351E-02

TABLE V

GOLD

PHI(R) CONTRIBUTIONS TO THE EFFECTIVE POTENTIAL
AND THE RADIAL WAVE FUNCTION. IONIZATION
ENERGY=.666 RYDBERGS. R IS IN UNITS OF 1/100
POHR UNITS.

R	PHI(R)	R(R)
51	.85920057E-01	-2.34182228E-02
52	.81550175E-01	-1.566848870E-02
53	.77242849E-01	-7.644916834E-03
54	.72997196E-01	4.332276630E-04
55	.688002431E-01	3.532002185E-03
56	.64677757E-01	1.655369603E-02
57	.60602264E-01	2.437482002E-02
58	.56581917E-01	3.197072205E-02
59	.52613558E-01	3.92581631E-02
60	.48696396E-01	4.617775106E-02
61	.44822106E-01	5.267592160E-02
62	.41010423E-01	5.87073474E-02
63	.37232139E-01	6.42325062E-02
64	.335114103E-01	6.92196808E-02
65	.29834210E-01	7.36395445E-02
66	.26192406E-01	7.74749069E-02
67	.22605683E-01	8.07108201E-02
68	.19055073E-01	8.33557302E-02
69	.15545643E-01	8.53519198E-02
70	.12076533E-01	8.67555079E-02
71	.086466347E-01	8.75537669E-02
72	.05255702E-01	8.77564259E-02
73	.01902593E-01	8.73772177E-02
74	.586476E-01	8.64328907E-02
75	.95306737E-01	8.49431246E-02
76	.92306267E-01	8.29306571E-02
77	.8805354E-01	8.04201721E-02
78	.83547979E-01	7.74333227E-02
79	.78253777E-01	7.401366281E-02
80	.72942989E-01	7.01755700E-02
81	.67635453E-01	6.59549043E-02
82	.62331113E-01	6.13830244E-02
83	.57029927E-01	5.64921140E-02
84	.516731370E-01	5.13142184E-02
85	.464367752E-01	4.582817256E-02
86	.412447164E-01	4.02263199E-02
87	.360956043E-01	3.433813705E-02
88	.309556925E-01	2.833767692E-02
89	.258660447E-01	2.22437877E-02
90	.208053106E-01	1.60124273E-02
91	.147377519E-01	9.71194595E-03
92	.84527038E-01	3.37021422E-03
93	.41904030E-01	2.99574624E-03
94	.29107370E-01	2.32834151E-03
95	.16436952E-01	1.56354651E-02
96	.933792401E-01	1.38164647E-02
97	.551117345E-01	2.00450280E-02
98	.35357967E-01	1.41047236E-02
99	.26010309E-01	1.00410953E-02
100	.2346632E-01	4.58356139E-02

TABLE V

GOLD

PHI(R) CONTRIBUTIONS TO THE EFFECTIVE POTENTIAL
AND THE RADIAL WAVE FUNCTION. IONIZATION
ENERGY=.666 RYDBERGS. R IS IN UNITS OF 1/100
BOHR UNITS.

R	PHI(R)	R(R)
101	2.20946541E-01	-5.14713601E-02
102	2.18450543E-01	-5.62326222E-02
103	2.15978254E-01	-6.22050389E-02
104	2.13529395E-01	-6.72755022E-02
105	2.11103607E-01	-7.21322040E-02
106	2.08700898E-01	-7.67645741E-02
107	2.06320743E-01	-8.11632556E-02
108	2.03962983E-01	-8.53260702E-02
109	2.01627376E-01	-8.92279802E-02
110	1.99231363E-01	-9.28910487E-02
111	1.97021684E-01	-9.62743968E-02
112	1.94751146E-01	-9.94041598E-02
113	1.92501852E-01	-1.02267442E-01
114	1.90273590E-01	-1.04862370E-01
115	1.88066153E-01	-1.07197547E-01
116	1.85879336E-01	-1.09243004E-01
117	1.83712943E-01	-1.11029156E-01
118	1.81566379E-01	-1.12547248E-01
119	1.79440657E-01	-1.13799221E-01
120	1.773334390E-01	-1.14787632E-01
121	1.75247799E-01	-1.15515689E-01
122	1.73180707E-01	-1.15987090E-01
123	1.71132941E-01	-1.16206076E-01
124	1.69104334E-01	-1.16177347E-01
125	1.67094718E-01	-1.15906026E-01
126	1.65103933E-01	-1.15327623E-01
127	1.63131220E-01	-1.14657990E-01
128	1.61173224E-01	-1.13769309E-01
129	1.59242993E-01	-1.12509972E-01
130	1.57325977E-01	-1.11111470E-01
131	1.55427072E-01	-1.09514368E-01
132	1.53546013E-01	-1.07716030E-01
133	1.51682780E-01	-1.05726895E-01
134	1.49837126E-01	-1.03554237E-01
135	1.48009124E-01	-1.01205622E-01
136	1.46198432E-01	-9.86893843E-02
137	1.44404991E-01	-9.60100955E-02
138	1.42622670E-01	-9.31783117E-02
139	1.40869345E-01	-9.02006702E-02
140	1.39126903E-01	-8.70844039E-02
141	1.37401100E-01	-8.38373014E-02
142	1.35692118E-01	-8.04667005E-02
143	1.33992559E-01	-7.69799690E-02
144	1.32323759E-01	-7.33843912E-02
145	1.30667352E-01	-6.96871554E-02
146	1.29019813E-01	-6.58953415E-02
147	1.27392167E-01	-6.20159103E-02
148	1.25780474E-01	-5.80556942E-02
149	1.24184625E-01	-5.40221387E-02
150	1.22604515E-01	-4.99195410E-02

TABLE V

GOLD

PHI(R) CONTRIBUTIONS TO THE EFFECTIVE POTENTIAL
AND THE RADIAL WAVE FUNCTION. IONIZATION
ENERGY=.666 RYDBERGS. R IS IN UNITS OF 1/100
BOHR UNITS.

R	PHI(R)	R(R)
151	1.21040041E-01	-4.57565509E-02
152	1.19491100E-01	-4.153865570E-02
153	1.17957591E-01	-3.72719353E-02
154	1.16432941E-01	-3.29622941E-02
155	1.149336439E-01	-2.86154701E-02
156	1.134486652E-01	-2.42370258E-02
157	1.11975894E-01	-1.98323465E-02
158	1.10519072E-01	-1.54066392E-02
159	1.09075103E-01	-1.09649509E-02
160	1.07646893E-01	-6.51206739E-03
161	1.062333351E-01	-2.05271628E-03
162	1.048324388E-01	-2.40233326E-03
163	1.034449214E-01	6.86769127E-03
164	1.02079941E-01	1.13203146E-02
165	1.00724081E-01	1.57623389E-02
166	9.93823493E-02	2.01906497E-02
167	9.80555159E-02	2.44009986E-02
168	9.67418269E-02	2.839901890E-02
169	9.54424697E-02	3.23548461E-02
170	9.41570017E-02	3.76920120E-02
171	9.28853441E-02	4.19927037E-02
172	9.16274114E-02	4.63972147E-02
173	9.03831332E-02	5.07097262E-02
174	8.91522419E-02	5.47089274E-02
175	8.79355193E-02	5.83967577E-02
176	8.67313222E-02	6.22983364E-02
177	8.55409021E-02	6.70543063E-02
178	8.436366790E-02	7.10739512E-02
179	8.321996358E-02	7.50542252E-02
180	8.204926971E-02	7.837998179E-02
181	8.09107978E-02	8.229537889E-02
182	7.97859335E-02	8.66747590E-02
183	7.86737602E-02	9.04414666E-02
184	7.75744947E-02	9.41527444E-02
185	7.64879639E-02	9.79076149E-02
186	7.54140936E-02	1.01405097E-01
187	7.435232179E-02	1.04944350E-01
188	7.330405935E-02	1.08424675E-01
189	7.22677495E-02	1.111945424E-01
190	7.124522176E-02	1.15206052E-01
191	7.023321936E-02	1.19506093E-01
192	6.923320021E-02	1.21745188E-01
193	6.82455920E-02	1.24923024E-01
194	6.72704756E-02	1.29039396E-01
195	6.63307393E-02	1.31094126E-01
196	6.53566274E-02	1.340827165E-01
197	6.44170526E-02	1.37019491E-01
198	6.34895693E-02	1.398882152E-01
199	6.25740307E-02	1.42696253E-01
200	6.16700973E-02	1.45442973E-01

TABLE V

GOLD

PHI(R) CONTRIBUTIONS TO THE EFFECTIVE POTENTIAL
AND THE RADIAL WAVE FUNCTION. IONIZATION
ENERGY=.666 RYDBERGS. R IS IN UNITS OF 1/100
BOHR UNITS.

R	PHI(R)	R(R)
201	6.07777941E-02	1.48129515E-01
202	5.98970551E-02	1.50753154E-01
203	5.90278148E-02	1.53317204E-01
204	5.81700079E-02	1.55821102E-01
205	5.73235696E-02	1.58265026E-01
206	5.64884352E-02	1.60649642E-01
207	5.56645403E-02	1.62979554E-01
208	5.48518209E-02	1.65242675E-01
209	5.40502131E-02	1.67445215E-01
210	5.32596544E-02	1.69604557E-01
211	5.24800735E-02	1.71692939E-01
212	5.17114252E-02	1.73772394E-01
213	5.09536309E-02	1.75772650E-01
214	5.02066322E-02	1.77692903E-01
215	4.94703637E-02	1.79552379E-01
216	4.87447764E-02	1.81356344E-01
217	4.80297939E-02	1.83112824E-01
218	4.73253597E-02	1.84837462E-01
219	4.66314120E-02	1.86530401E-01
220	4.59478907E-02	1.88192023E-01
221	4.52747117E-02	1.89826691E-01
222	4.46117769E-02	1.91420492E-01
223	4.39592643E-02	1.92976747E-01
224	4.33168346E-02	1.94499751E-01
225	4.26845261E-02	1.95984739E-01
226	4.20622791E-02	1.97436047E-01
227	4.14500634E-02	1.98859007E-01
228	4.08477729E-02	1.99233282E-01
229	4.02552071E-02	2.00555179E-01
230	3.96727071E-02	2.01868325E-01
231	3.90999970E-02	2.03180341E-01
232	3.85367366E-02	2.04397773E-01
233	3.79832479E-02	2.05619121E-01
234	3.74393446E-02	2.06836433E-01
235	3.69049632E-02	2.08050771E-01
236	3.63800600E-02	2.09262371E-01
237	3.58645615E-02	2.10471322E-01
238	3.53594114E-02	2.11677731E-01
239	3.48615599E-02	2.12881624E-01
240	3.43739404E-02	2.14083024E-01
241	3.38954978E-02	2.15281945E-01
242	3.34261174E-02	2.16478399E-01
243	3.29659912E-02	2.17672395E-01
244	3.25146533E-02	2.18863921E-01
245	3.20723408E-02	2.19952995E-01
246	3.16399171E-02	2.21040557E-01
247	3.12164324E-02	2.22126603E-01
248	3.07998506E-02	2.23211139E-01
249	3.03914052E-02	2.24294144E-01
250	2.99922965E-02	2.25375613E-01

TABLE V

GOLD

PHI(R) CONTRIBUTIONS TO THE EFFECTIVE POTENTIAL
AND THE RADIAL WAVE FUNCTION. IONIZATION
ENERGY=.666 RYDBERGS. R IS IN UNITS OF 1/100
BOHR UNITS.

R	PHI(R)	S(R)
251	.96031291E-02	2.17531632E-01
252	.92218392E-02	2.13091072E-01
253	.88490396E-02	2.12395092E-01
254	.84846737E-02	2.12764330E-01
255	.812966851E-02	2.13129932E-01
256	.77910177E-02	2.13443075E-01
257	.74416152E-02	2.13722917E-01
258	.71110421E-02	2.13900515E-01
259	.67873390E-02	2.14025923E-01
260	.64724373E-02	2.14049920E-01
261	.61655374E-02	2.14070404E-01
262	.58666617E-02	2.14088957E-01
263	.55755431E-02	2.14104777E-01
264	.52925139E-02	2.14122052E-01
265	.50173293E-02	2.14135452E-01
266	.47496996E-02	2.14147024E-01
267	.44899376E-02	2.14156699E-01
268	.42337710E-02	2.14164487E-01
269	.39933142E-02	2.14171236E-01
270	.37561119E-02	2.14175935E-01
271	.35226593E-02	2.14179066E-01
272	.33044483E-02	2.14180630E-01
273	.30899763E-02	2.14180630E-01
274	.28822866E-02	2.14179168E-01
275	.26833224E-02	2.14176248E-01
276	.24939933E-02	2.14171922E-01
277	.23035593E-02	2.14166621E-01
278	.21242955E-02	2.14159216E-01
279	.19533379E-02	2.14150980E-01
280	.17998792E-02	2.14141162E-01
281	.16311157E-02	2.14130275E-01
282	.14890415E-02	2.14118170E-01
283	.13336514E-02	2.14104887E-01
284	.11993393E-02	2.14090443E-01
285	.10699014E-02	2.14074883E-01
286	.99453101E-02	2.14059591E-01
287	.90828231E-02	2.14040355E-01
288	.80717723E-02	2.14022151E-01
289	.66137409E-02	2.14001639E-01
290	.55162224E-02	2.13980748E-01
291	.44251179E-02	2.13959864E-01
292	.33403754E-02	2.13938600E-01
293	.22619415E-02	2.13916219E-01
294	.01297641E-02	2.13897454E-01
295	.01237907E-02	2.13861762E-01
296	.006592691E-02	2.13835231E-01
297	.001024870E-02	2.13807784E-01
298	.99622572E-02	2.13779479E-01
299	.99203974E-02	2.13750029E-01
300	.99670061E-02	2.13720288E-01

TABLE V

GOLD

PHI(R) CONTRIBUTIONS TO THE EFFECTIVE POTENTIAL
AND THE RADIAL WAVE FUNCTION. IONIZATION
ENLRSY=.666 RYDBERGS. R IS IN UNITS OF 1/100
BOHR UNITS.

R	PHI(R)	R(R)
301	1.99341209E-02	2.168924401E-01
302	1.99013438E-02	2.16577666E-01
303	1.98686743E-02	2.16252205E-01
304	1.98361119E-02	2.15919941E-01
305	1.98036561E-02	2.15579192E-01
306	1.97711306E-02	2.15237069E-01
307	1.97390620E-02	2.14897455E-01
308	1.97069227E-02	2.14551089E-01
309	1.96748387E-02	2.14213983E-01
310	1.96429571E-02	2.13776150E-01
311	1.96111207E-02	2.13337599E-01
312	1.95794054E-02	2.12898344E-01
313	1.95477783E-02	2.12458365E-01
314	1.95162636E-02	2.12017765E-01
315	1.94848351E-02	2.11576464E-01
316	1.94535277E-02	2.11134504E-01
317	1.94223109E-02	2.10691996E-01
318	1.93911239E-02	2.10248650E-01
319	1.93600176E-02	2.10047791E-01
320	1.93292259E-02	2.09600292E-01
321	1.92984339E-02	2.09152011E-01
322	1.92677717E-02	2.08699516E-01
323	1.92370993E-02	2.08233247E-01
324	1.92065566E-02	2.07764070E-01
325	1.91761364E-02	2.07290040E-01
326	1.91458302E-02	2.06811049E-01
327	1.91155364E-02	2.06322552E-01
328	1.90853429E-02	2.05829352E-01
329	1.90553374E-02	2.05333974E-01
330	1.90255402E-02	2.04833913E-01
331	1.89959567E-02	2.04333350E-01
332	1.89665707E-02	2.03828295E-01
333	1.89373612E-02	2.03320752E-01
334	1.89083065E-02	2.02787488E-01
335	1.88793705E-02	2.02262754E-01
336	1.88505476E-02	2.01733499E-01
337	1.88218367E-02	2.01199779E-01
338	1.87932344E-02	2.00661717E-01
339	1.87647302E-02	2.00119396E-01
340	1.87363233E-02	1.99572903E-01
341	1.87080046E-02	1.99022333E-01
342	1.86797751E-02	1.98467777E-01
343	1.86516427E-02	1.97909304E-01
344	1.86235971E-02	1.97347022E-01
345	1.85956386E-02	1.96781009E-01
346	1.85677583E-02	1.96211351E-01
347	1.85399560E-02	1.95638013E-01
348	1.85122324E-02	1.95061436E-01
349	1.84845869E-02	1.94481345E-01
350	1.84570183E-02	1.93897941E-01

TABLE V.

GOLD

PHI(R) CONTRIBUTIONS TO THE EFFECTIVE POTENTIAL
AND THE RADIAL WAVE FUNCTION. IONIZATION
ENERGY=.666 RYDBERGS. R IS IN UNITS OF 1/100
BOHR UNITS.

R	PHI(R)	R(R)
351	1.84174625E-02	1.93311305E-01
352	1.83294798E-02	1.92721518E-01
353	1.83615919E-02	1.92128657E-01
354	1.83337636E-02	1.91532803E-01
355	1.83060394E-02	1.90934031E-01
356	1.82783940E-02	1.90333242E-01
357	1.82508319E-02	1.89728044E-01
358	1.82233529E-02	1.89120679E-01
359	1.81959356E-02	1.88511299E-01
360	1.81686423E-02	1.87899078E-01
361	1.81414110E-02	1.87284387E-01
362	1.81142502E-02	1.86666729E-01
363	1.80871899E-02	1.86047383E-01
364	1.80602002E-02	1.85426215E-01
365	1.80332922E-02	1.84802755E-01
366	1.80064539E-02	1.84176383E-01
367	1.79797199E-02	1.83548357E-01
368	1.79530459E-02	1.82918348E-01
369	1.79264536E-02	1.82286422E-01
370	1.78999043E-02	1.81652644E-01
371	1.78733519E-02	1.81017079E-01
372	1.78471531E-02	1.80379791E-01
373	1.78208773E-02	1.79740043E-01
374	1.77946763E-02	1.79100298E-01
375	1.77683536E-02	1.78458217E-01
376	1.77425006E-02	1.77814660E-01
377	1.77165334E-02	1.77169669E-01
378	1.76906406E-02	1.76523364E-01
379	1.76648212E-02	1.75875740E-01
380	1.76390773E-02	1.75226879E-01
381	1.76134093E-02	1.74575836E-01
382	1.75877813E-02	1.73922566E-01
383	1.75622936E-02	1.73267345E-01
384	1.75368474E-02	1.72620133E-01
385	1.75114743E-02	1.71965974E-01
386	1.74861755E-02	1.71310950E-01
387	1.74609249E-02	1.70654992E-01
388	1.74357955E-02	1.69999012E-01
389	1.74107143E-02	1.69344061E-01
390	1.73857051E-02	1.68688223E-01
391	1.73607676E-02	1.68033539E-01
392	1.73358901E-02	1.67378640E-01
393	1.73111067E-02	1.66704078E-01
394	1.72864392E-02	1.66043857E-01
395	1.72617729E-02	1.65382261E-01
396	1.72371459E-02	1.64721250E-01
397	1.72126324E-02	1.64059540E-01
398	1.71882189E-02	1.63397510E-01
399	1.71638914E-02	1.62733521E-01
400	1.71395503E-02	1.62072691E-01

TABLE V

COLE

PHI(R) CONTRIBUTIONS TO THE EFFECTIVE POTENTIAL
AND THE RADIAL WAVE FUNCTION. IONIZATION
ENERGY=.666 RYDBERGS. R IS IN UNITS OF 1/100
BOHR UNITS.

R	PHI(R)	R(R)
401	1.71152721E-02	1.61409999E-01
402	1.70911039E-02	1.60747159E-01
403	1.70670049E-02	1.60002423E-01
404	1.70429716E-02	1.59242125E-01
405	1.70190070E-02	1.58475827E-01
406	1.69951097E-02	1.57702532E-01
407	1.69712794E-02	1.56922551E-01
408	1.69475159E-02	1.56143255E-01
409	1.69238197E-02	1.55356967E-01
410	1.69001872E-02	1.54564463E-01
411	1.68766228E-02	1.53764844E-01
412	1.68531233E-02	1.52958120E-01
413	1.68296929E-02	1.52144288E-01
414	1.68063320E-02	1.51323260E-01
415	1.67830160E-02	1.50505095E-01
416	1.67597765E-02	1.49679837E-01
417	1.67366012E-02	1.48847514E-01
418	1.67134899E-02	1.48008155E-01
419	1.66904422E-02	1.47161751E-01
420	1.66674581E-02	1.46308300E-01
421	1.66445372E-02	1.45447809E-01
422	1.66216792E-02	1.44580276E-01
423	1.65988839E-02	1.43705709E-01
424	1.65761511E-02	1.42824094E-01
425	1.65534800E-02	1.41935580E-01
426	1.65308719E-02	1.41039125E-01
427	1.65083247E-02	1.40134782E-01
428	1.64858391E-02	1.39222541E-01
429	1.64634146E-02	1.38302402E-01
430	1.64410511E-02	1.37374363E-01
431	1.64187482E-02	1.36438425E-01
432	1.63965059E-02	1.35494588E-01
433	1.63743236E-02	1.34542852E-01
434	1.63522014E-02	1.33583216E-01
435	1.63301392E-02	1.32615680E-01
436	1.63081370E-02	1.31640243E-01
437	1.62861948E-02	1.30656905E-01
438	1.62643126E-02	1.29665667E-01
439	1.62424804E-02	1.28666529E-01
440	1.62207082E-02	1.27659491E-01
441	1.61990060E-02	1.26644553E-01
442	1.61773738E-02	1.25621715E-01
443	1.61557916E-02	1.24590977E-01
444	1.61342594E-02	1.23552339E-01
445	1.61127772E-02	1.22505801E-01
446	1.60913450E-02	1.21451363E-01
447	1.60699628E-02	1.20389025E-01
448	1.60486306E-02	1.19318787E-01
449	1.60273484E-02	1.18241649E-01
450	1.60061162E-02	1.17157611E-01

TABLE V

GOLD

PHI(R) CONTRIBUTIONS TO THE EFFECTIVE POTENTIAL
AND THE RADIAL WAVE FUNCTION. IONIZATION
ENERGY=.666 RYDBERGS. R IS IN UNITS OF 1/100
BOHR UNITS.

R	PHI(R)	R(R)
451	1.59850624E-02	1.28855760E-01
452	1.59639787E-02	1.28222947E-01
453	1.59429506E-02	1.27624576E-01
454	1.59219778E-02	1.26991079E-01
455	1.59010601E-02	1.26355900E-01
456	1.58800197E-02	1.25733364E-01
457	1.58593891E-02	1.25119122E-01
458	1.58386354E-02	1.24501472E-01
459	1.58179236E-02	1.23880525E-01
460	1.57972200E-02	1.23270536E-01
461	1.57766990E-02	1.22665734E-01
462	1.57561161E-02	1.22054568E-01
463	1.57356769E-02	1.21443557E-01
464	1.57152451E-02	1.20832703E-01
465	1.56949667E-02	1.20222000E-01
466	1.56745412E-02	1.19611471E-01
467	1.56540681E-02	1.19001096E-01
468	1.56334404E-02	1.18400833E-01
469	1.56132979E-02	1.17800834E-01
470	1.55933762E-02	1.17200949E-01
471	1.55735697E-02	1.16612311E-01
472	1.55538334E-02	1.16016304E-01
473	1.55339722E-02	1.15422982E-01
474	1.55143912E-02	1.14830958E-01
475	1.54949895E-02	1.14240443E-01
476	1.54747414E-02	1.13651748E-01
477	1.54545438E-02	1.13064782E-01
478	1.54343467E-02	1.12479066E-01
479	1.54141501E-02	1.11896092E-01
480	1.53939541E-02	1.11314379E-01
481	1.53737585E-02	1.10734416E-01
482	1.53535634E-02	1.10156310E-01
483	1.53333697E-02	1.09579951E-01
484	1.53131747E-02	1.09000539E-01
485	1.52929811E-02	1.08426264E-01
486	1.52727890E-02	1.07846171E-01
487	1.52525954E-02	1.07272260E-01
488	1.52324032E-02	1.06702533E-01
489	1.52122116E-02	1.06135990E-01
490	1.51920204E-02	1.05570632E-01
491	1.51718297E-02	1.05003459E-01
492	1.51516395E-02	1.04447473E-01
493	1.51314497E-02	1.03891474E-01
494	1.5111260504E-02	1.03336063E-01
495	1.51071703E-02	1.02800640E-01
496	1.50089337E-02	1.02254059E-01
497	1.50695512E-02	1.01703613E-01
498	1.50508126E-02	1.01155069E-01
499	1.50321199E-02	1.00609451E-01
500	1.50134736E-02	1.00063705E-01

TABLE V

GOLD

PHI(R) CONTRIBUTIONS TO THE EFFECTIVE POTENTIAL
AND THE RADIAL WAVE FUNCTION. IONIZATION
ENERGY=.666 RYDBERGS. R IS IN UNITS OF 1/100
BOHR UNITS.

R	PHI(R)	R(R)
501	1.49948735E-02	9.95208963E-02
502	1.49763195E-02	9.89800091E-02
503	1.49578113E-02	9.84410485E-02
504	1.49393488E-02	9.79040188E-02
505	1.49209318E-02	9.73689243E-02
506	1.49025602E-02	9.68357690E-02
507	1.48842337E-02	9.63045569E-02
508	1.48659523E-02	9.57752917E-02
509	1.48477157E-02	9.52479767E-02
510	1.48295238E-02	9.47226153E-02
511	1.48113765E-02	9.41992107E-02
512	1.47932735E-02	9.36777658E-02
513	1.47752147E-02	9.31582833E-02
514	1.47571999E-02	9.26407658E-02
515	1.47392290E-02	9.21252158E-02
516	1.47213018E-02	9.16116355E-02
517	1.47034182E-02	9.11000270E-02
518	1.46855790E-02	9.05903921E-02
519	1.46677810E-02	9.00827327E-02
520	1.46500271E-02	8.95770502E-02
521	1.46323162E-02	8.90733463E-02
522	1.46146480E-02	8.85716220E-02
523	1.45970224E-02	8.80718785E-02
524	1.45794393E-02	8.75741168E-02
525	1.45618984E-02	8.70783378E-02
526	1.45443998E-02	8.65845420E-02
527	1.45269431E-02	8.60927299E-02
528	1.45095283E-02	8.56029021E-02
529	1.44921552E-02	8.51150586E-02
530	1.44748237E-02	8.46291996E-02
531	1.44575336E-02	8.41453250E-02
532	1.44402847E-02	8.36634347E-02
533	1.44230769E-02	8.31835284E-02
534	1.44059101E-02	8.27056055E-02
535	1.43887841E-02	8.22296656E-02
536	1.43716988E-02	8.17557079E-02
537	1.43546540E-02	8.12837316E-02
538	1.43376496E-02	8.08137358E-02
539	1.43206854E-02	8.03457193E-02
540	1.43037614E-02	7.98796811E-02
541	1.42868772E-02	7.94156197E-02
542	1.42700329E-02	7.89535338E-02
543	1.42532283E-02	7.84934218E-02
544	1.42364632E-02	7.80352820E-02
545	1.42197375E-02	7.75791128E-02
546	1.42030510E-02	7.71249122E-02
547	1.41864037E-02	7.66726782E-02
548	1.41697953E-02	7.62224088E-02
549	1.41532258E-02	7.57741018E-02
550	1.41366950E-02	7.53277549E-02

TABLE V

GOLD

PHI(R) CONTRIBUTIONS TO THE EFFECTIVE POTENTIAL
AND THE RADIAL WAVE FUNCTION. IONIZATION
ENERGY=.666 RYDBERGS. R IS IN UNITS OF 1/100
BOHR UNITS.

R	PHI(R)	R(R)
551	1.41202028E-02	7.48833657E-02
552	1.41037489E-02	7.44409318E-02
553	1.40873334E-02	7.40004504E-02
554	1.40709561E-02	7.35619190E-02
555	1.40546168E-02	7.31253348E-02
556	1.40383154E-02	7.26906949E-02
557	1.40220518E-02	7.22579963E-02
558	1.40058258E-02	7.18272360E-02
559	1.39896373E-02	7.13984109E-02
560	1.39734862E-02	7.09715177E-02
561	1.39573724E-02	7.05465532E-02
562	1.39412256E-02	7.01235139E-02
563	1.39252559E-02	6.97023964E-02
564	1.39092530E-02	6.92831971E-02
565	1.38932869E-02	6.88659124E-02
566	1.38773574E-02	6.84505386E-02
567	1.38614643E-02	6.80370719E-02
568	1.38456077E-02	6.76255085E-02
569	1.38297872E-02	6.72158443E-02
570	1.38140029E-02	6.68080755E-02
571	1.37982546E-02	6.64021980E-02
572	1.37825421E-02	6.59982075E-02
573	1.37668654E-02	6.55960999E-02
574	1.37512243E-02	6.51958702E-02
575	1.37356187E-02	6.47975162E-02
576	1.37200048E-02	6.44010313E-02
577	1.37045135E-02	6.40064119E-02
578	1.36890137E-02	6.36136532E-02
579	1.36735489E-02	6.32227509E-02
580	1.36581190E-02	6.28337001E-02
581	1.36427239E-02	6.24464963E-02
582	1.36273634E-02	6.20611345E-02
583	1.36120375E-02	6.16776101E-02
584	1.35967461E-02	6.12959181E-02
585	1.35814889E-02	6.09160536E-02
586	1.35662660E-02	6.05380116E-02
587	1.35510771E-02	6.01617871E-02
588	1.35359223E-02	5.97873750E-02
589	1.35208012E-02	5.94147701E-02
590	1.35057140E-02	5.90439672E-02
591	1.34906603E-02	5.86749613E-02
592	1.34756402E-02	5.83077468E-02
593	1.34606535E-02	5.79423186E-02
594	1.34457001E-02	5.75786713E-02
595	1.34307798E-02	5.72167995E-02
596	1.34158927E-02	5.68566976E-02
597	1.34010385E-02	5.64983602E-02
598	1.33862172E-02	5.61417819E-02
599	1.33714286E-02	5.57869569E-02
600	1.33566726E-02	5.54338797E-02

TABLE V

GOLD

PHI(R) CONTRIBUTIONS TO THE EFFECTIVE POTENTIAL
AND THE RADIAL WAVE FUNCTION. IONIZATION
ENERGY=.666 RYDBERGS. R IS IN UNITS OF 1/100
BOHR UNITS.

R	PHI(R)	R(R)
601	1.33419492E-C2	5.50825447E-02
602	1.33272532E-C2	5.47329461E-02
603	1.33125996E-C2	5.43850783E-02
604	1.32979731E-C2	5.40389355E-02
605	1.32833787E-C2	5.36945118E-02
606	1.32688164E-C2	5.33518015E-02
607	1.32542859E-C2	5.30107987E-02
608	1.32397873E-C2	5.26714975E-02
609	1.32253203E-C2	5.23338921E-02
610	1.32108849E-C2	5.19979764E-02
611	1.31964909E-C2	5.16637444E-02
612	1.31821084E-C2	5.13311903E-02
613	1.31677671E-C2	5.10003079E-02
614	1.31534570E-C2	5.06710912E-02
615	1.31391780E-C2	5.03443534E-02
616	1.31249299E-C2	5.00176304E-02
617	1.31107127E-C2	4.96933741E-02
618	1.30965262E-C2	4.93707590E-02
619	1.30823705E-C2	4.90497789E-02
620	1.30682453E-C2	4.87304276E-02
621	1.30541506E-C2	4.84126989E-02
622	1.30400862E-C2	4.80965866E-02
623	1.30260521E-C2	4.77820843E-02
624	1.30120482E-C2	4.74691857E-02
625	1.29980744E-C2	4.71578847E-02
626	1.29841305E-C2	4.68481748E-02
627	1.29702165E-C2	4.65400497E-02
628	1.29563324E-C2	4.62335030E-02
629	1.29424779E-C2	4.59285284E-02
630	1.29286530E-C2	4.56251195E-02
631	1.29148576E-C2	4.53232699E-02
632	1.29010916E-C2	4.50229731E-02
633	1.28873550E-C2	4.47242228E-02
634	1.28736475E-C2	4.44270124E-02
635	1.28599692E-C2	4.41313355E-02
636	1.28463199E-C2	4.38371857E-02
637	1.28326996E-C2	4.35445564E-02
638	1.28191081E-C2	4.32534411E-02
639	1.28055454E-C2	4.29638334E-02
640	1.27920114E-C2	4.26757267E-02
641	1.27785059E-C2	4.23891144E-02
642	1.27650289E-C2	4.21039902E-02
643	1.27515803E-C2	4.18203473E-02
644	1.27381600E-C2	4.15381793E-02
645	1.27247680E-C2	4.12574796E-02
646	1.27114040E-C2	4.09782417E-02
647	1.26980682E-C2	4.07004588E-02
648	1.26847602E-C2	4.04241245E-02
649	1.26714801E-C2	4.01492322E-02
650	1.26582278E-C2	3.98757753E-02

TABLE V

GOLD

PHI(R) CONTRIBUTIONS TO THE EFFECTIVE POTENTIAL
AND THE RADIAL WAVE FUNCTION. IONIZATION
ENERGY=.666 RYDBERGS. R IS IN UNITS OF 1/100
BOHR UNITS.

R	PHI(R)	R(R)
651	1.26582278E-02	3.96037471E-02
652	1.26582278E-02	3.92331399E-02
653	1.26582278E-02	3.90639457E-02
654	1.26582278E-02	3.87961567E-02
655	1.26582278E-02	3.85297651E-02
656	1.26582278E-02	3.82647632E-02
657	1.26582278E-02	3.80011430E-02
658	1.26582278E-02	3.77388969E-02
659	1.26582278E-02	3.74780172E-02
660	1.26582278E-02	3.72184960E-02
661	1.26582278E-02	3.69603258E-02
662	1.26582278E-02	3.67034988E-02
663	1.26582278E-02	3.64480074E-02
664	1.26582278E-02	3.61938440E-02
665	1.26582278E-02	3.59410008E-02
666	1.26582278E-02	3.56894705E-02
667	1.26582278E-02	3.54392453E-02
668	1.26582278E-02	3.51903176E-02
669	1.26582278E-02	3.49426801E-02
670	1.26582278E-02	3.46963251E-02
671	1.26582278E-02	3.44512452E-02
672	1.26582278E-02	3.42074329E-02
673	1.26582278E-02	3.39648807E-02
674	1.26582278E-02	3.37233581E-02
675	1.26582278E-02	3.34833527E-02
676	1.26582278E-02	3.32447108E-02
677	1.26582278E-02	3.30071250E-02
678	1.26582278E-02	3.27707624E-02
679	1.26582278E-02	3.25356157E-02
680	1.26582278E-02	3.23016774E-02
681	1.26582278E-02	3.20689405E-02
682	1.26582278E-02	3.18373975E-02
683	1.26582278E-02	3.16070412E-02
684	1.26582278E-02	3.13778644E-02
685	1.26582278E-02	3.11498599E-02
686	1.26582278E-02	3.09230205E-02
687	1.26582278E-02	3.06973390E-02
688	1.26582278E-02	3.04728063E-02
689	1.26582278E-02	3.02494213E-02
690	1.26582278E-02	3.00271708E-02
691	1.26582278E-02	2.98060497E-02
692	1.26582278E-02	2.95860511E-02
693	1.26582278E-02	2.93671678E-02
694	1.26582278E-02	2.91493928E-02
695	1.26582278E-02	2.89327191E-02
696	1.26582278E-02	2.87171397E-02
697	1.26582278E-02	2.85026477E-02
698	1.26582278E-02	2.82892361E-02
699	1.26582278E-02	2.80768980E-02
700	1.26582278E-02	2.78656264E-02

TABLE V

GOLD

PHI(R) CONTRIBUTIONS TO THE EFFECTIVE POTENTIAL
AND THE RADIAL WAVE FUNCTION. IONIZATION
ENERGY=.666 RYDBERGS. R IS IN UNITS OF 1/100
BOHR UNITS.

R	PHI(R)	R(R)
701	1.265822278E-02	2.76554146E-02
702	1.265822278E-02	2.74462555E-02
703	1.265822278E-02	2.72381425E-02
704	1.265822278E-02	2.70310686E-02
705	1.265822278E-02	2.68250270E-02
706	1.265822278E-02	2.66200110E-02
707	1.265822278E-02	2.64160138E-02
708	1.265822278E-02	2.62130286E-02
709	1.265822278E-02	2.60110487E-02
710	1.265822278E-02	2.58100675E-02
711	1.265822278E-02	2.56100781E-02
712	1.265822278E-02	2.54110739E-02
713	1.265822278E-02	2.52130484E-02
714	1.265822278E-02	2.50159948E-02
715	1.265822278E-02	2.48199065E-02
716	1.265822278E-02	2.46247770E-02
717	1.265822278E-02	2.44305996E-02
718	1.265822278E-02	2.42373679E-02
719	1.265822278E-02	2.40450752E-02
720	1.265822278E-02	2.38537151E-02
721	1.265822278E-02	2.36632810E-02
722	1.265822278E-02	2.34737665E-02
723	1.265822278E-02	2.32851651E-02
724	1.265822278E-02	2.30974704E-02
725	1.265822278E-02	2.29106759E-02
726	1.265822278E-02	2.27247753E-02
727	1.265822278E-02	2.25397621E-02
728	1.265822278E-02	2.23556300E-02
729	1.265822278E-02	2.21723726E-02
730	1.265822278E-02	2.19899835E-02
731	1.265822278E-02	2.18084566E-02
732	1.265822278E-02	2.16277854E-02
733	1.265822278E-02	2.14479637E-02
734	1.265822278E-02	2.12689852E-02
735	1.265822278E-02	2.10908437E-02
736	1.265822278E-02	2.09135330E-02
737	1.265822278E-02	2.07370469E-02
738	1.265822278E-02	2.05613789E-02
739	1.265822278E-02	2.03865232E-02
740	1.265822278E-02	2.02124735E-02
741	1.265822278E-02	2.00392237E-02
742	1.265822278E-02	1.98667676E-02
743	1.265822278E-02	1.96950992E-02
744	1.265822278E-02	1.95242123E-02
745	1.265822278E-02	1.93541009E-02
746	1.265822278E-02	1.91847589E-02
747	1.265822278E-02	1.90161802E-02
748	1.265822278E-02	1.88483589E-02
749	1.265822278E-02	1.86812889E-02
750	1.265822278E-02	1.85149643E-02

TABLE V

GOLD

PHI(R) CONTRIBUTIONS TO THE EFFECTIVE POTENTIAL
AND THE RADIAL WAVE FUNCTION. IONIZATION
ENERGY=.666 RYDBERGS. R IS IN UNITS OF 1/100
BOHR UNITS.

R	PHI(R)	R(R)
751	1.26582278E-C2	1.83493791E-02
752	1.26582278E-02	1.81845272E-02
753	1.26582278E-02	1.80204028E-02
754	1.26582278E-02	1.78569999E-02
755	1.26582278E-02	1.76943127E-02
756	1.26582278E-02	1.75323351E-02
757	1.26582278E-02	1.73710614E-02
758	1.26582278E-C2	1.72104857E-02
759	1.26582278E-C2	1.70506021E-02
760	1.26582278E-02	1.68914047E-02
761	1.26582278E-02	1.67328878E-02
762	1.26582278E-C2	1.65750456E-02
763	1.26582278E-C2	1.64178722E-02
764	1.26582278E-02	1.62613619E-02
765	1.26582278E-C2	1.61055039E-02
766	1.26582278E-C2	1.59503075E-02
767	1.26582278E-C2	1.57957519E-02
768	1.26582278E-C2	1.56418365E-02
769	1.26582278E-C2	1.54885554E-02
770	1.26582278E-C2	1.53359031E-02
771	1.26582278E-C2	1.51838738E-02
772	1.26582278E-02	1.50324618E-02
773	1.26582278E-02	1.48816616E-02
774	1.26582278E-C2	1.47314675E-02
775	1.26582278E-02	1.45818738E-02
776	1.26582278E-02	1.44328750E-02
777	1.26582278E-C2	1.42844654E-02
778	1.26582278E-C2	1.41366395E-02
779	1.26582278E-02	1.39893916E-02
780	1.26582278E-02	1.38427163E-02
781	1.26582278E-C2	1.36966080E-02
782	1.26582278E-02	1.35510611E-02
783	1.26582278E-02	1.34060702E-02
784	1.26582278E-02	1.32616297E-02
785	1.26582278E-C2	1.31177341E-02
786	1.26582278E-02	1.29743779E-02
787	1.26582278E-02	1.28315557E-02
788	1.26582278E-02	1.26892619E-02
789	1.26582278E-C2	1.25474912E-02
790	1.26582278E-02	1.24062382E-02
791	1.26582278E-02	1.22654973E-02
792	1.26582278E-02	1.21252631E-02
793	1.26582278E-C2	1.19855303E-02
794	1.26582278E-02	1.18462934E-02
795	1.26582278E-02	1.17075472E-02
796	1.26582278E-C2	1.15692861E-02
797	1.26582278E-02	1.14315048E-02
798	1.26582278E-02	1.12941980E-02
799	1.26582278E-02	1.11573604E-02
800	1.26582278E-C2	1.10209865E-02

TABLE V

GOLD

PHI(R) CONTRIBUTIONS TO THE EFFECTIVE POTENTIAL
AND THE RADIAL WAVE FUNCTION. IONIZATION
ENERGY=.666 RYDBERGS. R IS IN UNITS OF 1/100
BOHR UNITS.

R	PHI(R)	R(R)
801	1.26582278E-02	1.08850711E-02
802	1.26582278E-02	1.07496089E-02
803	1.26582278E-02	1.06145945E-02
804	1.26582278E-02	1.04800227E-02
805	1.26582278E-02	1.03458882E-02
806	1.26582278E-02	1.02121856E-02
807	1.26582278E-02	1.00789098E-02
808	1.26582278E-02	9.94605545E-03
809	1.26582278E-02	9.81361731E-03
810	1.26582278E-02	9.68159016E-03
811	1.26582278E-02	9.54996874E-03
812	1.26582278E-02	9.41874784E-03
813	1.26582278E-02	9.28792224E-03
814	1.26582278E-02	9.15748674E-03
815	1.26582278E-02	9.02743612E-03
816	1.26582278E-02	8.89776519E-03
817	1.26582278E-02	8.76846878E-03
818	1.26582278E-02	8.63954169E-03
819	1.26582278E-02	8.51097876E-03
820	1.26582278E-02	8.38277483E-03
821	1.26582278E-02	8.25492473E-03
822	1.26582278E-02	8.12742331E-03
823	1.26582278E-02	8.00026543E-03
824	1.26582278E-02	7.87344596E-03
825	1.26582278E-02	7.74695975E-03
826	1.26582278E-02	7.62090168E-03
827	1.26582278E-02	7.49496664E-03
828	1.26582278E-02	7.36944950E-03
829	1.26582278E-02	7.24424517E-03
830	1.26582278E-02	7.11934853E-03

TIME, 1 MINUTES AND 4 SECONDS

TABLE VI

GOLD

VALUES FOR $\Psi(r)$ AND $\Psi(r)\Psi(r)^*$. R IN UNITS
OF 1/100 BOHR UNITS. IONIZATION ENERGY IS .666
RYDBERGS.

R	$\Psi(r)$	$\Psi(r)\Psi(r)^*$
1	7.63658744E-01	5.83174678E-01
2	1.40284349E+00	5.83174678E-01
3	9.90352310E-01	5.83174678E-01
4	4.66553645E-01	5.83174678E-01
5	3.59848971E-02	5.83174678E-01
6	-2.58283165E-01	5.83174678E-01
7	-4.25144424E-01	5.83174678E-01
8	-4.89410706E-01	5.83174678E-01
9	-4.78556795E-01	5.83174678E-01
10	-4.17480428E-01	5.83174678E-01
11	-3.26822316E-01	5.83174678E-01
12	-2.22654629E-01	5.83174678E-01
13	-1.16857130E-01	5.83174678E-01
14	-1.77268191E-02	5.83174678E-01
15	6.93608359E-02	5.83174678E-01
16	1.413227310E-01	5.83174678E-01
17	1.96841754E-01	5.83174678E-01
18	2.35854219E-01	5.83174678E-01
19	2.59221681E-01	5.83174678E-01
20	2.68378276E-01	5.83174678E-01
21	2.65146243E-01	5.83174678E-01
22	2.51505556E-01	5.83174678E-01
23	2.29483073E-01	5.83174678E-01
24	2.01050120E-01	5.83174678E-01
25	1.680555230E-01	5.83174678E-01
26	1.32180479E-01	5.83174678E-01
27	9.49161975E-02	5.83174678E-01
28	5.75495744E-02	5.83174678E-01
29	2.11632936E-02	5.83174678E-01
30	-1.33566016E-02	5.83174678E-01
31	-4.53121926E-02	5.83174678E-01
32	-7.41753143E-02	5.83174678E-01
33	-9.95747190E-02	5.83174678E-01
34	-1.21273023E-01	5.83174678E-01
35	-1.29153846E-01	5.83174678E-01
36	-1.53201830E-01	5.83174678E-01
37	-1.63486841E-01	5.83174678E-01
38	-1.70148003E-01	5.83174678E-01
39	-1.73320099E-01	5.83174678E-01
40	-1.73420430E-01	5.83174678E-01
41	-1.70537799E-01	5.83174678E-01
42	-1.65021995E-01	5.83174678E-01
43	-1.57175632E-01	5.83174678E-01
44	-1.47306497E-01	5.83174678E-01
45	-1.35721350E-01	5.83174678E-01
46	-1.22720798E-01	5.83174678E-01
47	-1.08595022E-01	5.83174678E-01
48	-9.36205320E-02	5.83174678E-01
49	-7.80575737E-02	5.83174678E-01
50	-6.21482701E-02	5.83174678E-01

TABLE VI

GOLD

VALUES FOR $\Psi(R)$ AND $\Psi(R)\Psi(R)^*$. R IN UNITS
OF 1/100 BOHR UNITS. IONIZATION ENERGY IS .666
RYDBERGS.

R	$\Psi(R)$	$\Psi(R)\Psi(R)^*$
51	-4.61153389E-02	5.83174678E-01
52	-3.01613211E-02	5.83174678E-01
53	-1.44682421E-02	5.83174678E-01
54	8.02364129E-04	5.83174678E-01
55	1.55091306E-02	5.83174678E-01
56	2.95302871E-02	5.83174678E-01
57	4.27628251E-02	5.83174678E-01
58	5.51219316E-02	5.83174678E-01
59	6.65392594E-02	5.83174678E-01
60	7.69625176E-02	5.83174678E-01
61	8.63539606E-02	5.83174678E-01
62	9.46893699E-02	5.83174678E-01
63	1.01956359E-01	5.83174678E-01
64	1.08154199E-01	5.83174678E-01
65	1.13291607E-01	5.83174678E-01
66	1.17586212E-01	5.83174678E-01
67	1.20463337E-01	5.83174678E-01
68	1.22554337E-01	5.83174678E-01
69	1.23692435E-01	5.83174678E-01
70	1.23936440E-01	5.83174678E-01
71	1.23315163E-01	5.83174678E-01
72	1.21684972E-01	5.83174678E-01
73	1.19694319E-01	5.83174678E-01
74	1.16801071E-01	5.83174678E-01
75	1.13257499E-01	5.83174678E-01
76	1.09119226E-01	5.83174678E-01
77	1.04441722E-01	5.83174678E-01
78	9.92799778E-02	5.83174678E-01
79	9.36881369E-02	5.83174678E-01
80	8.77194625E-02	5.83174678E-01
81	8.14258094E-02	5.83174678E-01
82	7.48574322E-02	5.83174678E-01
83	6.80627890E-02	5.83174678E-01
84	6.10883552E-02	5.83174678E-01
85	5.39785009E-02	5.83174678E-01
86	4.67753720E-02	5.83174678E-01
87	3.95188166E-02	5.83174678E-01
88	3.22467236E-02	5.83174678E-01
89	2.49930154E-02	5.83174678E-01
90	1.77915864E-02	5.83174678E-01
91	1.06723582E-02	5.83174678E-01
92	3.66327633E-03	5.83174678E-01
93	-3.21004972E-03	5.83174678E-01
94	-9.92429948E-03	5.83174678E-01
95	-1.64583394E-02	5.83174678E-01
96	-2.27933321E-02	5.83174678E-01
97	-2.89124619E-02	5.83174678E-01
98	-3.48008002E-02	5.83174678E-01
99	-4.04455407E-02	5.83174678E-01
100	-4.58356139E-02	5.83174678E-01

TABLE VI

GOLD

VALUES FOR $\Psi(R)$ AND $\Psi(R)\Psi(R)^*$. R IN UNITS
OF 1/100 BOHR UNITS. IONIZATION ENERGY IS .666
RYDBERGS.

R	$\Psi(R)$	$\Psi(R)\Psi(R)^*$
101	-5.09617427E-02	5.83174678E-01
102	-5.53163031E-02	5.83174678E-01
103	-6.03932417E-02	5.83174678E-01
104	-6.46879829E-02	5.83174678E-01
105	-6.86973372E-02	5.83174678E-01
106	-7.24194096E-02	5.83174678E-01
107	-7.58535029E-02	5.83174678E-01
108	-7.90000650E-02	5.83174678E-01
109	-8.18605322E-02	5.83174678E-01
110	-8.44373170E-02	5.83174678E-01
111	-8.67336908E-02	5.83174678E-01
112	-8.87537141E-02	5.83174678E-01
113	-9.05021609E-02	5.83174678E-01
114	-9.19844473E-02	5.83174678E-01
115	-9.32065626E-02	5.83174678E-01
116	-9.41750038E-02	5.83174678E-01
117	-9.48967141E-02	5.83174678E-01
118	-9.53790237E-02	5.83174678E-01
119	-9.56295939E-02	5.83174678E-01
120	-9.56563661E-02	5.83174678E-01
121	-9.54675113E-02	5.83174678E-01
122	-9.50713852E-02	5.83174678E-01
123	-9.44764849E-02	5.83174678E-01
124	-9.36914091E-02	5.83174678E-01
125	-9.27249209E-02	5.83174678E-01
126	-9.15854143E-02	5.83174678E-01
127	-9.02818917E-02	5.83174678E-01
128	-8.88228857E-02	5.83174678E-01
129	-8.72170324E-02	5.83174678E-01
130	-8.54728474E-02	5.83174678E-01
131	-8.35987539E-02	5.83174678E-01
132	-8.16030528E-02	5.83174678E-01
133	-7.94939057E-02	5.83174678E-01
134	-7.72793184E-02	5.83174678E-01
135	-7.49671276E-02	5.83174678E-01
136	-7.25649885E-02	5.83174678E-01
137	-7.00803639E-02	5.83174678E-01
138	-6.75205158E-02	5.83174678E-01
139	-6.48924971E-02	5.83174678E-01
140	-6.22031456E-02	5.83174678E-01
141	-5.94590720E-02	5.83174678E-01
142	-5.66666905E-02	5.83174678E-01
143	-5.38321461E-02	5.83174678E-01
144	-5.09617328E-02	5.83174678E-01
145	-4.80601073E-02	5.83174678E-01
146	-4.51337955E-02	5.83174678E-01
147	-4.21876941E-02	5.83174678E-01
148	-3.92262204E-02	5.83174678E-01
149	-3.62559651E-02	5.83174678E-01
150	-3.32796940E-02	5.83174678E-01

TABLE VI

GOLD

VALUES FOR $\Psi(r)$ AND $\Psi(r) \Psi(r)^*$. r IN UNITS OF 1/100 BOHR UNITS. IONIZATION ENERGY IS .666 RYDBERGS.

R	$\Psi(r)$	$\Psi(r) \Psi(r)^*$
151	-3.03023516E-02	5.83174678E-01
152	-2.73280638E-02	5.83174678E-01
153	-2.43607420E-02	5.83174678E-01
154	-2.14040871E-02	5.83174678E-01
155	-1.84615236E-02	5.83174678E-01
156	-1.55365550E-02	5.83174678E-01
157	-1.26320678E-02	5.83174678E-01
158	-9.75103744E-03	5.83174678E-01
159	-6.82618288E-03	5.83174678E-01
160	-4.07004243E-03	5.83174678E-01
161	-1.27497905E-03	5.83174678E-01
162	1.48681398E-03	5.83174678E-01
163	4.21370753E-03	5.83174678E-01
164	6.90263024E-03	5.83174678E-01
165	9.55306596E-03	5.83174678E-01
166	1.21630420E-02	5.83174678E-01
167	1.47311296E-02	5.83174678E-01
168	1.72560331E-02	5.83174678E-01
169	1.97365953E-02	5.83174678E-01
170	2.21717718E-02	5.83174678E-01
171	2.45606454E-02	5.83174678E-01
172	2.69024114E-02	5.83174678E-01
173	2.91963735E-02	5.83174678E-01
174	3.14419395E-02	5.83174678E-01
175	3.36386158E-02	5.83174678E-01
176	3.57860025E-02	5.83174678E-01
177	3.78857939E-02	5.83174678E-01
178	3.99317485E-02	5.83174678E-01
179	4.19297343E-02	5.83174678E-01
180	4.38776766E-02	5.83174678E-01
181	4.57755740E-02	5.83174678E-01
182	4.76234939E-02	5.83174678E-01
183	4.94215664E-02	5.83174678E-01
184	5.11699806E-02	5.83174678E-01
185	5.28689210E-02	5.83174678E-01
186	5.45198638E-02	5.83174678E-01
187	5.61199735E-02	5.83174678E-01
188	5.76726296E-02	5.83174678E-01
189	5.91774732E-02	5.83174678E-01
190	6.06347641E-02	5.83174678E-01
191	6.20450776E-02	5.83174678E-01
192	6.34089519E-02	5.83174678E-01
193	6.47269553E-02	5.83174678E-01
194	6.59996234E-02	5.83174678E-01
195	6.72277569E-02	5.83174678E-01
196	6.84118190E-02	5.83174678E-01
197	6.95525335E-02	5.83174678E-01
198	7.06505819E-02	5.83174678E-01
199	7.17066622E-02	5.83174678E-01
200	7.27214863E-02	5.83174678E-01

TABLE VI

GOLD

VALUES FOR $\Psi(R)$ AND $\Psi(R)\Psi(R)^*$. R IN UNITS
OF 1/100 BOHR UNITS. IONIZATION ENERGY IS .666
RYDBERGS.

R	$\Psi(R)$	$\Psi(R)\Psi(R)^*$
201	7.36957737E-02	5.83174678E-01
202	7.46302741E-02	5.83174678E-01
203	7.55257165E-02	5.83174678E-01
204	7.63828568E-02	5.83174678E-01
205	7.72024519E-02	5.83174678E-01
206	7.79852632E-02	5.83174678E-01
207	7.87320551E-02	5.83174678E-01
208	7.94433939E-02	5.83174678E-01
209	8.01206465E-02	5.83174678E-01
210	8.07639795E-02	5.83174678E-01
211	8.13743579E-02	5.83174678E-01
212	8.19525444E-02	5.83174678E-01
213	8.24992933E-02	5.83174678E-01
214	8.30153732E-02	5.83174678E-01
215	8.35015250E-02	5.83174678E-01
216	8.39584224E-02	5.83174678E-01
217	8.43837015E-02	5.83174678E-01
218	8.47878266E-02	5.83174678E-01
219	8.51616497E-02	5.83174678E-01
220	8.55091978E-02	5.83174678E-01
221	8.58311814E-02	5.83174678E-01
222	8.61282279E-02	5.83174678E-01
223	8.64012369E-02	5.83174678E-01
224	8.66506799E-02	5.83174678E-01
225	8.68772861E-02	5.83174678E-01
226	8.70817260E-02	5.83174678E-01
227	8.72646439E-02	5.83174678E-01
228	8.74266777E-02	5.83174678E-01
229	8.75684539E-02	5.83174678E-01
230	8.76905881E-02	5.83174678E-01
231	8.77936843E-02	5.83174678E-01
232	8.78783360E-02	5.83174678E-01
233	8.79451239E-02	5.83174678E-01
234	8.79946180E-02	5.83174678E-01
235	8.80273768E-02	5.83174678E-01
236	8.80439454E-02	5.83174678E-01
237	8.80448601E-02	5.83174678E-01
238	8.80306434E-02	5.83174678E-01
239	8.80018067E-02	5.83174678E-01
240	8.79582501E-02	5.83174678E-01
241	8.79022615E-02	5.83174678E-01
242	8.78325179E-02	5.83174678E-01
243	8.77500845E-02	5.83174678E-01
244	8.76554151E-02	5.83174678E-01
245	8.75489524E-02	5.83174678E-01
246	8.74311279E-02	5.83174678E-01
247	8.73023618E-02	5.83174678E-01
248	8.71630637E-02	5.83174678E-01
249	8.70136320E-02	5.83174678E-01
250	8.68544547E-02	5.83174678E-01

TABLE VI

GOLD

VALUES FOR $\Psi(r)$ AND $\Psi(r)\Psi(r)^*$. r IN UNITS
OF 1/100 BOHR UNITS. IONIZATION ENERGY IS .666
RYDBERGS.

r	$\Psi(r)$	$\Psi(r)\Psi(r)^*$
251	8.6685909CE-02	5.87174678E-01
252	8.65087619E-02	5.87174678E-01
253	8.63221699E-02	5.87174678E-01
254	8.61276795E-02	5.87174678E-01
255	8.59252271E-02	5.87174678E-01
256	8.57151375E-02	5.87174678E-01
257	8.54977336E-02	5.87174678E-01
258	8.52733169E-02	5.87174678E-01
259	8.50421876E-02	5.87174678E-01
260	8.48046346E-02	5.87174678E-01
261	8.45609380E-02	5.87174678E-01
262	8.43113689E-02	5.87174678E-01
263	8.40561399E-02	5.87174678E-01
264	8.37956546E-02	5.87174678E-01
265	8.35300090E-02	5.87174678E-01
266	8.32594904E-02	5.87174678E-01
267	8.29843285E-02	5.87174678E-01
268	8.27047448E-02	5.87174678E-01
269	8.24209534E-02	5.87174678E-01
270	8.21331608E-02	5.87174678E-01
271	8.18415668E-02	5.87174678E-01
272	8.15463661E-02	5.87174678E-01
273	8.12477323E-02	5.87174678E-01
274	8.09458569E-02	5.87174678E-01
275	8.06409052E-02	5.87174678E-01
276	8.03330441E-02	5.87174678E-01
277	8.00224316E-02	5.87174678E-01
278	7.97092204E-02	5.87174678E-01
279	7.93933556E-02	5.87174678E-01
280	7.90755915E-02	5.87174678E-01
281	7.87554291E-02	5.87174678E-01
282	7.84332290E-02	5.87174678E-01
283	7.81109105E-02	5.87174678E-01
284	7.77831735E-02	5.87174678E-01
285	7.74555538E-02	5.87174678E-01
286	7.71263482E-02	5.87174678E-01
287	7.67956622E-02	5.87174678E-01
288	7.64635943E-02	5.87174678E-01
289	7.61302394E-02	5.87174678E-01
290	7.57956942E-02	5.87174678E-01
291	7.54600169E-02	5.87174678E-01
292	7.51233317E-02	5.87174678E-01
293	7.47856632E-02	5.87174678E-01
294	7.44471242E-02	5.87174678E-01
295	7.41107773E-02	5.87174678E-01
296	7.37676724E-02	5.87174678E-01
297	7.34263849E-02	5.87174678E-01
298	7.30854633E-02	5.87174678E-01
299	7.27433476E-02	5.87174678E-01
300	7.24009621E-02	5.87174678E-01

TABLE VI

GOLD

VALUES FOR $\Psi(r)$ AND $\Psi(r)\Psi(r)^*$. r IN UNITS
OF 1/100 BOHR UNITS. IONIZATION ENERGY IS .666
RYDBERGS.

R	$\Psi(r)$	$\Psi(r)\Psi(r)^*$
301	7.20579406E-02	5.83174678E-01
302	7.17144589E-02	5.83174678E-01
303	7.13705627E-02	5.83174678E-01
304	7.10262265E-02	5.83174678E-01
305	7.06817041E-02	5.83174678E-01
306	7.03368285E-02	5.83174678E-01
307	6.99917117E-02	5.83174678E-01
308	6.96463950E-02	5.83174678E-01
309	6.93009137E-02	5.83174678E-01
310	6.89553224E-02	5.83174678E-01
311	6.86096450E-02	5.83174678E-01
312	6.82639244E-02	5.83174678E-01
313	6.79181979E-02	5.83174678E-01
314	6.75725018E-02	5.83174678E-01
315	6.72268720E-02	5.83174678E-01
316	6.68811343E-02	5.83174678E-01
317	6.65359499E-02	5.83174678E-01
318	6.61907225E-02	5.83174678E-01
319	6.58455702E-02	5.83174678E-01
320	6.55003913E-02	5.83174678E-01
321	6.51553297E-02	5.83174678E-01
322	6.48102161E-02	5.83174678E-01
323	6.44650925E-02	5.83174678E-01
324	6.41199713E-02	5.83174678E-01
325	6.37748506E-02	5.83174678E-01
326	6.34297290E-02	5.83174678E-01
327	6.30846074E-02	5.83174678E-01
328	6.27394857E-02	5.83174678E-01
329	6.23943641E-02	5.83174678E-01
330	6.20492425E-02	5.83174678E-01
331	6.17041209E-02	5.83174678E-01
332	6.13589993E-02	5.83174678E-01
333	6.10138777E-02	5.83174678E-01
334	6.06687561E-02	5.83174678E-01
335	6.03236345E-02	5.83174678E-01
336	6.00039728E-02	5.83174678E-01
337	5.97031935E-02	5.83174678E-01
338	5.94024142E-02	5.83174678E-01
339	5.91016349E-02	5.83174678E-01
340	5.88008556E-02	5.83174678E-01
341	5.85000763E-02	5.83174678E-01
342	5.82000763E-02	5.83174678E-01
343	5.79000763E-02	5.83174678E-01
344	5.76000763E-02	5.83174678E-01
345	5.73000763E-02	5.83174678E-01
346	5.70000763E-02	5.83174678E-01
347	5.67000763E-02	5.83174678E-01
348	5.64000763E-02	5.83174678E-01
349	5.61000763E-02	5.83174678E-01
350	5.58000763E-02	5.83174678E-01

TABLE VI

GOLD

VALUES FOR $\Psi_1(R)$ AND $\Psi_1(R) \Psi_1(R)^*$. R IN UNITS
OF 1/100 BOHR UNITS. IONIZATION ENERGY IS .666
RYDBERGS.

R	$\Psi_1(R)$	$\Psi_1(R) \Psi_1(R)^*$
351	5.507444460E-02	5.83174678E-01
352	5.47504312E-02	5.83174678E-01
353	5.44273217E-02	5.83174678E-01
354	5.41053115E-02	5.83174678E-01
355	5.37842342E-02	5.83174678E-01
356	5.34641629E-02	5.83174678E-01
357	5.31451104E-02	5.83174678E-01
358	5.28270892E-02	5.83174678E-01
359	5.25101112E-02	5.83174678E-01
360	5.21941883E-02	5.83174678E-01
361	5.18793316E-02	5.83174678E-01
362	5.15655523E-02	5.83174678E-01
363	5.12528610E-02	5.83174678E-01
364	5.09412679E-02	5.83174678E-01
365	5.06307830E-02	5.83174678E-01
366	5.03214161E-02	5.83174678E-01
367	5.00131763E-02	5.83174678E-01
368	4.97060729E-02	5.83174678E-01
369	4.94001144E-02	5.83174678E-01
370	4.90953092E-02	5.83174678E-01
371	4.87916656E-02	5.83174678E-01
372	4.84891912E-02	5.83174678E-01
373	4.81878937E-02	5.83174678E-01
374	4.78877802E-02	5.83174678E-01
375	4.75888577E-02	5.83174678E-01
376	4.72911311E-02	5.83174678E-01
377	4.69946126E-02	5.83174678E-01
378	4.66993024E-02	5.83174678E-01
379	4.64052085E-02	5.83174678E-01
380	4.61123365E-02	5.83174678E-01
381	4.58206919E-02	5.83174678E-01
382	4.55302798E-02	5.83174678E-01
383	4.52411051E-02	5.83174678E-01
384	4.49531726E-02	5.83174678E-01
385	4.46664956E-02	5.83174678E-01
386	4.43810515E-02	5.83174678E-01
387	4.40968713E-02	5.83174678E-01
388	4.38139498E-02	5.83174678E-01
389	4.35322905E-02	5.83174678E-01
390	4.32518968E-02	5.83174678E-01
391	4.29727720E-02	5.83174678E-01
392	4.26949190E-02	5.83174678E-01
393	4.24183405E-02	5.83174678E-01
394	4.21430392E-02	5.83174678E-01
395	4.18690175E-02	5.83174678E-01
396	4.15962775E-02	5.83174678E-01
397	4.13248212E-02	5.83174678E-01
398	4.10546506E-02	5.83174678E-01
399	4.07857674E-02	5.83174678E-01
400	4.05181729E-02	5.83174678E-01

TABLE VI

GOLD

VALUES FOR $\Psi(r)$ AND $\Psi(r)\Psi(r)^* \cdot r$ IN UNITS
OF 1/100 ROHR UNITS. IONIZATION ENERGY IS .666
RYDBERGS.

R	$\Psi(r)$	$\Psi(r)\Psi(r)^* \cdot r$
401	4.02518685E-02	5.83174678E-01
402	3.99868555E-02	5.83174678E-01
403	3.97231347E-02	5.83174678E-01
404	3.94607071E-02	5.83174678E-01
405	3.91995734E-02	5.83174678E-01
406	3.89397340E-02	5.83174678E-01
407	3.86811894E-02	5.83174678E-01
408	3.84232398E-02	5.83174678E-01
409	3.81672854E-02	5.83174678E-01
410	3.79133260E-02	5.83174678E-01
411	3.76599616E-02	5.83174678E-01
412	3.74078917E-02	5.83174678E-01
413	3.71571160E-02	5.83174678E-01
414	3.69076339E-02	5.83174678E-01
415	3.66594447E-02	5.83174678E-01
416	3.64125473E-02	5.83174678E-01
417	3.61669517E-02	5.83174678E-01
418	3.59226317E-02	5.83174678E-01
419	3.56795924E-02	5.83174678E-01
420	3.54378339E-02	5.83174678E-01
421	3.51974406E-02	5.83174678E-01
422	3.49582337E-02	5.83174678E-01
423	3.47203352E-02	5.83174678E-01
424	3.44837486E-02	5.83174678E-01
425	3.42484244E-02	5.83174678E-01
426	3.40143778E-02	5.83174678E-01
427	3.37816070E-02	5.83174678E-01
428	3.35501027E-02	5.83174678E-01
429	3.33200339E-02	5.83174678E-01
430	3.30909227E-02	5.83174678E-01
431	3.28632372E-02	5.83174678E-01
432	3.26368115E-02	5.83174678E-01
433	3.24116477E-02	5.83174678E-01
434	3.21877429E-02	5.83174678E-01
435	3.19650247E-02	5.83174678E-01
436	3.17433700E-02	5.83174678E-01
437	3.15233556E-02	5.83174678E-01
438	3.13046603E-02	5.83174678E-01
439	3.10877009E-02	5.83174678E-01
440	3.08706005E-02	5.83174678E-01
441	3.06554301E-02	5.83174678E-01
442	3.04414255E-02	5.83174678E-01
443	3.02287227E-02	5.83174678E-01
444	3.00017319E-02	5.83174678E-01
445	2.97807071E-02	5.83174678E-01
446	2.95598045E-02	5.83174678E-01
447	2.93390237E-02	5.83174678E-01
448	2.91183645E-02	5.83174678E-01
449	2.89782643E-02	5.83174678E-01
450	2.87740911E-02	5.83174678E-01

TABLE VI

GOLD

VALUES FOR $\Psi(r)$ AND $\Psi(r)\Psi(r)^*$. r IN UNITS
OF $1/100$ BOHR UNITS. IONIZATION ENERGY IS .666
RYDBERGS.

R	$\Psi(r)$	$\Psi(r)\Psi(r)^*$
451	2.85711219E-02	5.83174678E-01
452	2.83693550E-02	5.83174678E-01
453	2.81687800E-02	5.83174678E-01
454	2.79694000E-02	5.83174678E-01
455	2.77712099E-02	5.83174678E-01
456	2.75742027E-02	5.83174678E-01
457	2.73783768E-02	5.83174678E-01
458	2.71837271E-02	5.83174678E-01
459	2.69902508E-02	5.83174678E-01
460	2.67979425E-02	5.83174678E-01
461	2.66067989E-02	5.83174678E-01
462	2.64168146E-02	5.83174678E-01
463	2.62279265E-02	5.83174678E-01
464	2.60403100E-02	5.83174678E-01
465	2.58537807E-02	5.83174678E-01
466	2.56683944E-02	5.83174678E-01
467	2.54841467E-02	5.83174678E-01
468	2.53010331E-02	5.83174678E-01
469	2.51190422E-02	5.83174678E-01
470	2.49381206E-02	5.83174678E-01
471	2.47584529E-02	5.83174678E-01
472	2.45798314E-02	5.83174678E-01
473	2.44023210E-02	5.83174678E-01
474	2.42259193E-02	5.83174678E-01
475	2.40506195E-02	5.83174678E-01
476	2.38764177E-02	5.83174678E-01
477	2.37033094E-02	5.83174678E-01
478	2.35312999E-02	5.83174678E-01
479	2.33602545E-02	5.83174678E-01
480	2.31904985E-02	5.83174678E-01
481	2.30221717E-02	5.83174678E-01
482	2.28544006E-02	5.83174678E-01
483	2.26873605E-02	5.83174678E-01
484	2.25211775E-02	5.83174678E-01
485	2.23557245E-02	5.83174678E-01
486	2.21937676E-02	5.83174678E-01
487	2.20317357E-02	5.83174678E-01
488	2.18699452E-02	5.83174678E-01
489	2.17095914E-02	5.83174678E-01
490	2.15502696E-02	5.83174678E-01
491	2.13919749E-02	5.83174678E-01
492	2.12347022E-02	5.83174678E-01
493	2.10784447E-02	5.83174678E-01
494	2.09232045E-02	5.83174678E-01
495	2.07699697E-02	5.83174678E-01
496	2.06157377E-02	5.83174678E-01
497	2.04635037E-02	5.83174678E-01
498	2.03122628E-02	5.83174678E-01
499	2.01620103E-02	5.83174678E-01
500	2.00127410E-02	5.83174678E-01

TABLE VI

GOLD

VALUES FOR $\Psi(r)$ AND $\Psi(r)\Psi(r)^*$. r IN UNITS
OF 1/100 BOHR UNITS. IONIZATION ENERGY IS .666
RYDBERGS.

R	$\Psi(r)$	$\Psi(r)\Psi(r)^*$
501	1.98644504E-02	5.83174678E-01
502	1.97171333E-02	5.83174678E-01
503	1.95707850E-02	5.83174678E-01
504	1.94254006E-02	5.83174678E-01
505	1.92809751E-02	5.83174678E-01
506	1.91375038E-02	5.83174678E-01
507	1.89949816E-02	5.83174678E-01
508	1.88534039E-02	5.83174678E-01
509	1.87127656E-02	5.83174678E-01
510	1.85730618E-02	5.83174678E-01
511	1.84342878E-02	5.83174678E-01
512	1.82964338E-02	5.83174678E-01
513	1.81595509E-02	5.83174678E-01
514	1.80233495E-02	5.83174678E-01
515	1.78883914E-02	5.83174678E-01
516	1.77541929E-02	5.83174678E-01
517	1.76208895E-02	5.83174678E-01
518	1.74889492E-02	5.83174678E-01
519	1.73586981E-02	5.83174678E-01
520	1.72296355E-02	5.83174678E-01
521	1.70996611E-02	5.83174678E-01
522	1.69667745E-02	5.83174678E-01
523	1.68339747E-02	5.83174678E-01
524	1.67012617E-02	5.83174678E-01
525	1.65696350E-02	5.83174678E-01
526	1.64380939E-02	5.83174678E-01
527	1.63066381E-02	5.83174678E-01
528	1.61762670E-02	5.83174678E-01
529	1.60469803E-02	5.83174678E-01
530	1.59187773E-02	5.83174678E-01
531	1.57916579E-02	5.83174678E-01
532	1.56656209E-02	5.83174678E-01
533	1.55406665E-02	5.83174678E-01
534	1.54167941E-02	5.83174678E-01
535	1.52937003E-02	5.83174678E-01
536	1.51712529E-02	5.83174678E-01
537	1.50493063E-02	5.83174678E-01
538	1.49278114E-02	5.83174678E-01
539	1.48067144E-02	5.83174678E-01
540	1.46860535E-02	5.83174678E-01
541	1.45658794E-02	5.83174678E-01
542	1.44461451E-02	5.83174678E-01
543	1.43269055E-02	5.83174678E-01
544	1.42081172E-02	5.83174678E-01
545	1.40897369E-02	5.83174678E-01
546	1.39717190E-02	5.83174678E-01
547	1.38540193E-02	5.83174678E-01
548	1.37366919E-02	5.83174678E-01
549	1.36197820E-02	5.83174678E-01
550	1.35032355E-02	5.83174678E-01

TABLE VI

GOLD

VALUES FOR $\Psi(r)$ AND $\Psi(r) \Psi(r)^*$. r IN UNITS
OF $1/100$ BOHR UNITS. IONIZATION ENERGY IS .666
RYDBERGS.

R	$\Psi(r)$	$\Psi(r) \Psi(r)^*$
551	1.35904475E-02	5.522174678E-01
552	1.34856760E-02	5.522174678E-01
553	1.33816366E-02	5.522174678E-01
554	1.32783247E-02	5.522174678E-01
555	1.31757360E-02	5.522174678E-01
556	1.30738660E-02	5.522174678E-01
557	1.29727103E-02	5.522174678E-01
558	1.28722264E-02	5.522174678E-01
559	1.27725243E-02	5.522174678E-01
560	1.26734953E-02	5.522174678E-01
561	1.25751432E-02	5.522174678E-01
562	1.24774936E-02	5.522174678E-01
563	1.23805322E-02	5.522174678E-01
564	1.22842544E-02	5.522174678E-01
565	1.21886571E-02	5.522174678E-01
566	1.20937347E-02	5.522174678E-01
567	1.19994938E-02	5.522174678E-01
568	1.19058994E-02	5.522174678E-01
569	1.18129779E-02	5.522174678E-01
570	1.17207130E-02	5.522174678E-01
571	1.16291065E-02	5.522174678E-01
572	1.15379149E-02	5.522174678E-01
573	1.14473335E-02	5.522174678E-01
574	1.13558166E-02	5.522174678E-01
575	1.12649133E-02	5.522174678E-01
576	1.11740733E-02	5.522174678E-01
577	1.10822961E-02	5.522174678E-01
578	1.10005922E-02	5.522174678E-01
579	1.09193302E-02	5.522174678E-01
580	1.08322396E-02	5.522174678E-01
581	1.07449106E-02	5.522174678E-01
582	1.06633429E-02	5.522174678E-01
583	1.05793499E-02	5.522174678E-01
584	1.04958764E-02	5.522174678E-01
585	1.04113006E-02	5.522174678E-01
586	1.03307137E-02	5.522174678E-01
587	1.02492026E-02	5.522174678E-01
588	1.01673220E-02	5.522174678E-01
589	1.00875972E-02	5.522174678E-01
590	1.00074521E-02	5.522174678E-01
591	9.92808143E-03	5.522174678E-01
592	9.84928136E-03	5.522174678E-01
593	9.77104367E-03	5.522174678E-01
594	9.69337901E-03	5.522174678E-01
595	9.61626332E-03	5.522174678E-01
596	9.53971436E-03	5.522174678E-01
597	9.46371193E-03	5.522174678E-01
598	9.38825734E-03	5.522174678E-01
599	9.31354840E-03	5.522174678E-01
600	9.23897996E-03	5.522174678E-01

TABLE VI

GOLD

VALUES FOR $\Psi(r)$ AND $\Psi(r)\Psi(r)^*$. r IN UNITS
OF $1/100$ BOHR UNITS. IONIZATION ENERGY IS .666
RYDBERGS.

r	$\Psi(r)$	$\Psi(r)\Psi(r)^*$
601	9.16514987E-03	5.822174679E-01
602	9.09105152E-03	5.822174679E-01
603	9.01902430E-03	5.822174679E-01
604	8.94682436E-03	5.822174679E-01
605	8.87512591E-03	5.822174679E-01
606	8.80392764E-03	5.822174679E-01
607	8.73324525E-03	5.822174679E-01
608	8.66307525E-03	5.822174679E-01
609	8.59341413E-03	5.822174679E-01
610	8.52425842E-03	5.822174679E-01
611	8.45560465E-03	5.822174679E-01
612	8.38744493E-03	5.822174679E-01
613	8.31972221E-03	5.822174679E-01
614	8.25262071E-03	5.822174679E-01
615	8.18594049E-03	5.822174679E-01
616	8.11974519E-03	5.822174679E-01
617	8.05403146E-03	5.822174679E-01
618	7.98892959E-03	5.822174679E-01
619	7.92440357E-03	5.822174679E-01
620	7.85997463E-03	5.822174679E-01
621	7.79592257E-03	5.822174679E-01
622	7.73257019E-03	5.822174679E-01
623	7.66967645E-03	5.822174679E-01
624	7.60722413E-03	5.822174679E-01
625	7.54526155E-03	5.822174679E-01
626	7.48383399E-03	5.822174679E-01
627	7.42226534E-03	5.822174679E-01
628	7.36202377E-03	5.822174679E-01
629	7.30180322E-03	5.822174679E-01
630	7.24202447E-03	5.822174679E-01
631	7.18227689E-03	5.822174679E-01
632	7.12332991E-03	5.822174679E-01
633	7.06543204E-03	5.822174679E-01
634	7.00741520E-03	5.822174679E-01
635	6.94998165E-03	5.822174679E-01
636	6.89263999E-03	5.822174679E-01
637	6.83588201E-03	5.822174679E-01
638	6.77953360E-03	5.822174679E-01
639	6.72360050E-03	5.822174679E-01
640	6.66808229E-03	5.822174679E-01
641	6.61296663E-03	5.822174679E-01
642	6.55822539E-03	5.822174679E-01
643	6.50399420E-03	5.822174679E-01
644	6.45000279E-03	5.822174679E-01
645	6.39655008E-03	5.822174679E-01
646	6.34333321E-03	5.822174679E-01
647	6.29006422E-03	5.822174679E-01
648	6.23733220E-03	5.822174679E-01
649	6.18632222E-03	5.822174679E-01
650	6.13473466E-03	5.822174679E-01

TABLE VI

GOLD

VALUES FOR $\Psi(r)$ AND $\Psi(r)\Psi(r)^*$. R IN UNITS
OF 1/100 BOHR UNITS. IONIZATION ENERGY IS .666
RYDBERGS.

R	$\Psi(r)$	$\Psi(r)\Psi(r)^*$
651	6.08352491E-03	5.83174678E-01
652	6.032269017E-03	5.83174678E-01
653	5.98222752E-03	5.83174678E-01
654	5.93213406E-03	5.83174678E-01
655	5.88240639E-03	5.83174678E-01
656	5.83304316E-03	5.83174678E-01
657	5.78404003E-03	5.83174678E-01
658	5.73532467E-03	5.83174678E-01
659	5.68710427E-03	5.83174678E-01
660	5.63916606E-03	5.83174678E-01
661	5.59157727E-03	5.83174678E-01
662	5.54433517E-03	5.83174678E-01
663	5.49743701E-03	5.83174678E-01
664	5.45088011E-03	5.83174678E-01
665	5.40466617E-03	5.83174678E-01
666	5.35877935E-03	5.83174678E-01
667	5.31323017E-03	5.83174678E-01
668	5.26801162E-03	5.83174678E-01
669	5.22312109E-03	5.83174678E-01
670	5.17855599E-03	5.83174678E-01
671	5.13431374E-03	5.83174678E-01
672	5.09039130E-03	5.83174678E-01
673	5.04678763E-03	5.83174678E-01
674	5.00349370E-03	5.83174678E-01
675	4.96052253E-03	5.83174678E-01
676	4.91785560E-03	5.83174678E-01
677	4.87549853E-03	5.83174678E-01
678	4.83334457E-03	5.83174678E-01
679	4.79169597E-03	5.83174678E-01
680	4.75024668E-03	5.83174678E-01
681	4.70909552E-03	5.83174678E-01
682	4.66824010E-03	5.83174678E-01
683	4.62767807E-03	5.83174678E-01
684	4.58740708E-03	5.83174678E-01
685	4.54742430E-03	5.83174678E-01
686	4.50772394E-03	5.83174678E-01
687	4.46831718E-03	5.83174678E-01
688	4.42918726E-03	5.83174678E-01
689	4.39033369E-03	5.83174678E-01
690	4.35176328E-03	5.83174678E-01
691	4.31346595E-03	5.83174678E-01
692	4.27544091E-03	5.83174678E-01
693	4.23768654E-03	5.83174678E-01
694	4.20020063E-03	5.83174678E-01
695	4.16298116E-03	5.83174678E-01
696	4.12603583E-03	5.83174678E-01
697	4.08933225E-03	5.83174678E-01
698	4.05289916E-03	5.83174678E-01
699	4.01672360E-03	5.83174678E-01
700	3.98080378E-03	5.83174678E-01

TABLE VI

GOLD

VALUES FOR $\Psi(r)$ AND $\Psi(r) \Psi(r)^*$. r IN UNITS
OF 1/100 BOHR UNITS. IONIZATION ENERGY IS .666
RYDPERGS.

R	$\Psi(r)$	$\Psi(r) \Psi(r)^*$
701	.94513760E-03	5.83174678E-01
702	.90972301E-03	5.83174678E-01
703	.87455797E-03	5.83174678E-01
704	.83964043E-03	5.83174678E-01
705	.80496837E-03	5.83174678E-01
706	.77053931E-03	5.83174678E-01
707	.73635273E-03	5.83174678E-01
708	.70240517E-03	5.83174678E-01
709	.66869517E-03	5.83174678E-01
710	.63522077E-03	5.83174678E-01
711	.60198004E-03	5.83174678E-01
712	.56897106E-03	5.83174678E-01
713	.53619192E-03	5.83174678E-01
714	.50364072E-03	5.83174678E-01
715	.47131559E-03	5.83174678E-01
716	.43922146E-03	5.83174678E-01
717	.40733360E-03	5.83174678E-01
718	.37567799E-03	5.83174678E-01
719	.34433355E-03	5.83174678E-01
720	.31330159E-03	5.83174678E-01
721	.28252022E-03	5.83174678E-01
722	.25200631E-03	5.83174678E-01
723	.22200631E-03	5.83174678E-01
724	.19025934E-03	5.83174678E-01
725	.16000232E-03	5.83174678E-01
726	.13013434E-03	5.83174678E-01
727	.10037293E-03	5.83174678E-01
728	.70828294E-03	5.83174678E-01
729	.40414777E-03	5.83174678E-01
730	.10127265E-03	5.83174678E-01
731	.98337299E-03	5.83174678E-01
732	.95461549E-03	5.83174678E-01
733	.92605236E-03	5.83174678E-01
734	.89763191E-03	5.83174678E-01
735	.86955025E-03	5.83174678E-01
736	.84151263E-03	5.83174678E-01
737	.81371059E-03	5.83174678E-01
738	.78602470E-03	5.83174678E-01
739	.75866349E-03	5.83174678E-01
740	.73141534E-03	5.83174678E-01
741	.70434826E-03	5.83174678E-01
742	.67744619E-03	5.83174678E-01
743	.65075335E-03	5.83174678E-01
744	.62422208E-03	5.83174678E-01
745	.59786589E-03	5.83174678E-01
746	.57168334E-03	5.83174678E-01
747	.54566733E-03	5.83174678E-01
748	.51983340E-03	5.83174678E-01
749	.49416402E-03	5.83174678E-01
750	.46866191E-03	5.83174678E-01

TABLE VI

GOLD

VALUES FOR $\Psi(r)$ AND $\Psi(r)\Psi(r)^*$. r IN UNITS
OF 1/100 BOHR UNITS. IONIZATION ENERGY IS .666
RYDBERGS.

r	$\Psi(r)$	$\Psi(r)\Psi(r)^*$
751	2.44332611E-03	5.83174673E-01
752	2.41915521E-03	5.83174673E-01
753	2.39314773E-03	5.83174673E-01
754	2.36683023E-03	5.83174673E-01
755	2.34361757E-03	5.83174673E-01
756	2.31909195E-03	5.83174673E-01
757	2.29472410E-03	5.83174673E-01
758	2.27051262E-03	5.83174673E-01
759	2.24645561E-03	5.83174673E-01
760	2.22255325E-03	5.83174673E-01
761	2.19880261E-03	5.83174673E-01
762	2.17520293E-03	5.83174673E-01
763	2.15175233E-03	5.83174673E-01
764	2.12845051E-03	5.83174673E-01
765	2.10529539E-03	5.83174673E-01
766	2.08227553E-03	5.83174673E-01
767	2.05940007E-03	5.83174673E-01
768	2.03666974E-03	5.83174673E-01
769	2.01411144E-03	5.83174673E-01
770	1.99167573E-03	5.83174673E-01
771	1.96937400E-03	5.83174673E-01
772	1.94721009E-03	5.83174673E-01
773	1.92519261E-03	5.83174673E-01
774	1.90329037E-03	5.83174673E-01
775	1.88153210E-03	5.83174673E-01
776	1.85990657E-03	5.83174673E-01
777	1.83838412E-03	5.83174673E-01
778	1.81704877E-03	5.83174673E-01
779	1.79589140E-03	5.83174673E-01
780	1.77477072E-03	5.83174673E-01
781	1.75372702E-03	5.83174673E-01
782	1.73287227E-03	5.83174673E-01
783	1.71214179E-03	5.83174673E-01
784	1.69153440E-03	5.83174673E-01
785	1.67104092E-03	5.83174673E-01
786	1.65068421E-03	5.83174673E-01
787	1.63043209E-03	5.83174673E-01
788	1.61031242E-03	5.83174673E-01
789	1.59030307E-03	5.83174673E-01
790	1.57040989E-03	5.83174673E-01
791	1.55063176E-03	5.83174673E-01
792	1.53096756E-03	5.83174673E-01
793	1.51141618E-03	5.83174673E-01
794	1.49197650E-03	5.83174673E-01
795	1.47264744E-03	5.83174673E-01
796	1.45342790E-03	5.83174673E-01
797	1.43431679E-03	5.83174673E-01
798	1.41531304E-03	5.83174673E-01
799	1.39641557E-03	5.83174673E-01
800	1.37762331E-03	5.83174673E-01

TABLE VI

GOLD

VALUES FOR $\Psi(r)$ AND $\Psi(r) \Psi(r)^*$. r IN UNITS
OF 1/100 BOHR UNITS. IONIZATION ENERGY IS .666
RYDBERGS.

r	$\Psi(r)$	$\Psi(r) \Psi(r)^*$
801	1.358935522E-03	5.82174678E-01
802	1.340355024E-03	5.82174678E-01
803	1.322186731E-03	5.82174678E-01
804	1.303748541E-03	5.82174678E-01
805	1.28520330E-03	5.82174678E-01
806	1.267000055E-03	5.82174678E-01
807	1.248935554E-03	5.82174678E-01
808	1.230947461E-03	5.82174678E-01
809	1.21305529E-03	5.82174678E-01
810	1.19525804E-03	5.82174678E-01
811	1.17755472E-03	5.82174678E-01
812	1.15994433E-03	5.82174678E-01
813	1.14242586E-03	5.82174678E-01
814	1.12499287E-03	5.82174678E-01
815	1.10766087E-03	5.82174678E-01
816	1.09041240E-03	5.82174678E-01
817	1.07325199E-03	5.82174678E-01
818	1.05617863E-03	5.82174678E-01
819	1.03919155E-03	5.82174678E-01
820	1.02222226E-03	5.82174678E-01
821	1.00547123E-03	5.82174678E-01
822	9.8876762E-04	5.82174678E-01
823	9.7208571E-04	5.82174678E-01
824	9.5551528E-04	5.82174678E-01
825	9.3902542E-04	5.82174678E-01
826	9.2261521E-04	5.82174678E-01
827	9.0628375E-04	5.82174678E-01
828	8.9003013E-04	5.82174678E-01
829	8.7385745E-04	5.82174678E-01
830	8.5775283E-04	5.82174678E-01

TIME, 1 MINUTES AND 2 SECONDS

TABLE VII

GOLD

LOWEST ENERGY STATE IS 1.194 RYDBERGS. RADIAL WAVE
R(R) AND PSI(R) WITH R IN 1/100 BOHR UNITS

R	R(R)	PSI(R)
1	7.63668275E-03	7.63668275E-01
2	2.80575038E-02	1.40287519E+00
3	2.97277998E-02	9.90926660E-01
4	1.86657869E-02	4.66644673E-01
5	1.80550235E-03	3.61100469E-02
6	-1.54903306E-02	-2.58172176E-01
7	-2.97551698E-02	-4.25073854E-01
8	-3.91526554E-02	-4.89408193E-01
9	-4.30755542E-02	-4.78617269E-01
10	-4.17613016E-02	-4.17613016E-01
11	-3.59724647E-02	-3.27022406E-01
12	-2.67490334E-02	-2.22908361E-01
13	-1.52291669E-02	-1.17147438E-01
14	-2.52462309E-03	-1.80330221E-02
15	1.035590390E-02	6.90602598E-02
16	2.25685805E-02	1.41053628E-01
17	3.34243650E-02	1.26613912E-01
18	4.24240319E-02	2.35699066E-01
19	4.92342486E-02	2.59127624E-01
20	5.36749065E-02	2.69337453E-01
21	5.56990276E-02	2.65233463E-01
22	5.53707721E-02	2.51695328E-01
23	5.28432372E-02	2.29753205E-01
24	4.83372020E-02	2.01400009E-01
25	4.21215599E-02	1.68496236E-01
26	3.44958656E-02	1.32267640E-01
27	2.57752255E-02	9.54637930E-02
28	1.62775400E-02	5.91340716E-02
29	6.31306601E-03	2.17691932E-02
30	-3.82386553E-03	-1.27462184E-02
31	-1.38611567E-02	-4.47134088E-02
32	-2.35544909E-02	-7.36046597E-02
33	-3.26853428E-02	-9.90464935E-02
34	-4.10726750E-02	-1.20080193E-01
35	-4.85635272E-02	-1.33875293E-01
36	-5.50377017E-02	-1.52888250E-01
37	-6.04057212E-02	-1.64255970E-01
38	-6.46072234E-02	-1.70019000E-01
39	-6.76089932E-02	-1.73356238E-01
40	-6.94023367E-02	-1.73505584E-01
41	-7.00011679E-02	-1.70734556E-01
42	-6.94387872E-02	-1.65330446E-01
43	-6.77655374E-02	-1.57594273E-01
44	-6.50461299E-02	-1.47832113E-01
45	-6.13571126E-02	-1.36354913E-01
46	-5.67844555E-02	-1.23444469E-01
47	-5.14212821E-02	-1.09406993E-01
48	-4.53657666E-02	-9.45120153E-02
49	-3.87192099E-02	-7.90187957E-02
50	-3.15843903E-02	-6.31686006E-02

TABLE VII

GOLD

LOWEST ENERGY STATE IS 1.194 RYDBERGS. RADIAL WAVE
R(R) AND PSI(R) WITH R IN 1/100 BOHR. UNITS

R	R(R)	PSI(R)
51	-2.406355632E-02	-4.71834572E-02
52	-1.62579263E-02	-3.12653776E-02
53	-8.26588762E-03	-1.55960144E-02
54	-1.81806782E-04	-3.56672225E-04
55	7.90423651E-03	1.43713339E-02
56	1.52074793E-02	2.84062130E-02
57	2.37489474E-02	4.16648192E-02
58	3.13558647E-02	5.40661835E-02
59	3.86619419E-02	6.55287150E-02
60	4.56075555E-02	7.60125625E-02
61	5.21392307E-02	8.54751323E-02
62	5.82126372E-02	9.39913503E-02
63	6.37865110E-02	1.01248430E-01
64	6.88285110E-02	1.07544548E-01
65	7.33120207E-02	1.12787724E-01
66	7.72165040E-02	1.16994703E-01
67	8.05272240E-02	1.20189887E-01
68	8.32349306E-02	1.22404310E-01
69	8.53555268E-02	1.23674676E-01
70	8.68297160E-02	1.24404245E-01
71	8.77226449E-02	1.23555302E-01
72	8.80235253E-02	1.22225489E-01
73	8.77452762E-02	1.20199003E-01
74	8.69041468E-02	1.17438033E-01
75	8.55193603E-02	1.14025814E-01
76	8.36127579E-02	1.10016787E-01
77	8.12084566E-02	1.05465522E-01
78	7.83305199E-02	1.00442630E-01
79	7.50126373E-02	9.49527055E-02
80	7.12778342E-02	8.90972922E-02
81	6.71581779E-02	8.29113307E-02
82	6.26845160E-02	7.64445317E-02
83	5.78882270E-02	6.97448518E-02
84	5.28009235E-02	6.28583196E-02
85	4.74545642E-02	5.58223899E-02
86	4.18806081E-02	4.86983815E-02
87	3.61104961E-02	4.15063058E-02
88	3.01751147E-02	3.42899031E-02
89	2.41104216E-02	2.70840632E-02
90	1.79291898E-02	1.99213220E-02
91	1.16762975E-02	1.28331865E-02
92	5.37606551E-03	5.84334947E-03
93	-9.46901277E-04	-1.01306589E-03
94	-7.26589159E-03	-7.72267191E-03
95	-1.35566476E-02	-1.42701553E-02
96	-1.97957131E-02	-2.06205345E-02
97	-2.59609717E-02	-2.67638283E-02
98	-3.20315738E-02	-3.26852793E-02
99	-3.79879556E-02	-3.83716724E-02
100	-4.38118491E-02	-4.38118491E-02

TABLE VII

GOLD

LOWEST ENERGY STATE IS 1.194 RYDBERGS. RADIAL WAVE
R(R) AND PSI(R) WITH R IN 1/100 BOHR UNITS

R	R(R)	PSI(R)
101	-4.94862342E-02	-4.89963210E-02
102	-5.49955839E-02	-5.39172391E-02
103	-6.03253537E-02	-5.85683046E-02
104	-6.54624646E-02	-6.29446775E-02
105	-7.03950312E-02	-6.70426869E-02
106	-7.51123356E-02	-7.08607411E-02
107	-7.96050469E-02	-7.43972401E-02
108	-8.38646879E-02	-7.76524688E-02
109	-8.78840982E-02	-8.06276130E-02
110	-9.16571455E-02	-8.33246777E-02
111	-9.51787342E-02	-8.57466074E-02
112	-9.84447631E-02	-8.78971099E-02
113	-1.01452081E-01	-8.97806025E-02
114	-1.04199442E-01	-9.14021417E-02
115	-1.06682459E-01	-9.27673559E-02
116	-1.08903562E-01	-9.38823808E-02
117	-1.10861245E-01	-9.47537990E-02
118	-1.12558526E-01	-9.53828581E-02
119	-1.13994901E-01	-9.57940342E-02
120	-1.15173295E-01	-9.59777454E-02
121	-1.16096522E-01	-9.59475395E-02
122	-1.16767240E-01	-9.57114262E-02
123	-1.17191410E-01	-9.53775637E-02
124	-1.17371251E-01	-9.49542344E-02
125	-1.17312204E-01	-9.39497634E-02
126	-1.17019392E-01	-9.23722337E-02
127	-1.16498222E-01	-9.17309370E-02
128	-1.15754646E-01	-9.04333169E-02
129	-1.14794532E-01	-8.89880092E-02
130	-1.13624227E-01	-8.74032251E-02
131	-1.12250227E-01	-8.56871960E-02
132	-1.10679203E-01	-8.38478809E-02
133	-1.08917977E-01	-8.18932156E-02
134	-1.06973491E-01	-7.98309636E-02
135	-1.04852794E-01	-7.76627291E-02
136	-1.02562965E-01	-7.54139449E-02
137	-1.00111190E-01	-7.30732616E-02
138	-9.75046439E-02	-7.06555390E-02
139	-9.47505148E-02	-6.81658380E-02
140	-9.18559798E-02	-6.56114141E-02
141	-8.88281251E-02	-6.29987122E-02
142	-8.56742301E-02	-6.03339648E-02
143	-8.24011524E-02	-5.76231835E-02
144	-7.90159141E-02	-5.48721629E-02
145	-7.55253985E-02	-5.20864742E-02
146	-7.19363490E-02	-4.92714719E-02
147	-6.82554531E-02	-4.64322944E-02
148	-6.44892582E-02	-4.35733823E-02
149	-6.06441627E-02	-4.07007903E-02
150	-5.67264484E-02	-3.78176323E-02

TABLE VII

GOLD

LOWEST ENERGY STATE IS 1.194 RYDBERGS. RADIAL WAVE
R(R) AND PSI(R) WITH R IN 1/100 BOHR UNITS

R	R(R)	PSI(R)
151	-5.27422428E-02	-3.49286416E-02
152	-4.86975479E-02	-3.20378605E-02
153	-4.45981753E-02	-2.91491342E-02
154	-4.04498017E-02	-2.62661050E-02
155	-3.62579348E-02	-2.33922160E-02
156	-3.20272170E-02	-2.05307160E-02
157	-2.77649222E-02	-1.76894663E-02
158	-2.34739546E-02	-1.48356933E-02
159	-1.91598467E-02	-1.20502181E-02
160	-1.48272594E-02	-9.26703711E-03
161	-1.04806208E-02	-6.50973965E-03
162	-6.12442718E-03	-3.78051061E-03
163	-1.76264290E-03	-1.09213759E-03
164	2.60069864E-03	1.58579185E-03
165	6.96179293E-03	4.21926844E-03
166	1.13170073E-02	6.81747214E-03
167	1.56628607E-02	9.37895852E-03
168	1.99060574E-02	1.19024151E-02
169	2.43134483E-02	1.43866558E-02
170	2.86120474E-02	1.68330616E-02
171	3.28390242E-02	1.92333475E-02
172	3.71417013E-02	2.15940124E-02
173	4.13675511E-02	2.39116793E-02
174	4.55641929E-02	2.61863177E-02
175	4.97293887E-02	2.84187935E-02
176	5.38610406E-02	3.06028640E-02
177	5.79571867E-02	3.27441733E-02
178	6.20159976E-02	3.48404481E-02
179	6.60357728E-02	3.68991493E-02
180	7.00149336E-02	3.88997187E-02
181	7.39520354E-02	4.08957478E-02
182	7.78457322E-02	4.27723903E-02
183	8.16948041E-02	4.46441269E-02
184	8.54981334E-02	4.64663796E-02
185	8.92547284E-02	4.82457991E-02
186	9.29636699E-02	4.99804677E-02
187	9.66241574E-02	5.16706724E-02
188	1.00235430E-01	5.33167449E-02
189	1.03797020E-01	5.49190582E-02
190	1.07320324E-01	5.64780234E-02
191	1.10769707E-01	5.79940875E-02
192	1.14178041E-01	5.94677298E-02
193	1.17535958E-01	6.089994600E-02
194	1.20842241E-01	6.22899215E-02
195	1.24092674E-01	6.36393576E-02
196	1.27299398E-01	6.49486726E-02
197	1.30450181E-01	6.62183659E-02
198	1.33549143E-01	6.74490621E-02
199	1.36596320E-01	6.86414020E-02
200	1.39592093E-01	6.97960415E-02

TABLE VII

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LOWEST ENERGY STATE IS 1.194 RYDBERGS. RADIAL WAVE
R(R) AND PSI(R) WITH R IN 1/100 BOHR UNITS

R	R(R)	PSI(R)
201	1.42536435E-01	7.09136493E-02
202	1.45429709E-01	7.19942051E-02
203	1.48272212E-01	7.30404984E-02
204	1.51064298E-01	7.40511266E-02
205	1.53806363E-01	7.50274940E-02
206	1.56498938E-01	7.59703099E-02
207	1.59142195E-01	7.68800287E-02
208	1.61736937E-01	7.77581423E-02
209	1.64283601E-01	7.86045937E-02
210	1.66782752E-01	7.94203582E-02
211	1.69234995E-01	8.02061540E-02
212	1.71640919E-01	8.09626975E-02
213	1.74001196E-01	8.16907025E-02
214	1.76316433E-01	8.23900890E-02
215	1.78587465E-01	8.30639372E-02
216	1.80814844E-01	8.37105760E-02
217	1.82999342E-01	8.43331423E-02
218	1.85141693E-01	8.49273219E-02
219	1.87242646E-01	8.54989250E-02
220	1.89302962E-01	8.60466001E-02
221	1.91323341E-01	8.65716802E-02
222	1.93304730E-01	8.70742253E-02
223	1.95247332E-01	8.75550205E-02
224	1.97153424E-01	8.80149215E-02
225	1.99022299E-01	8.84543557E-02
226	2.00855282E-01	8.88740184E-02
227	2.02653182E-01	8.92745296E-02
228	2.04416813E-01	8.96564968E-02
229	2.06146987E-01	9.00205183E-02
230	2.07844519E-01	9.03667182E-02
231	2.09510223E-01	9.06970662E-02
232	2.11144912E-01	9.10107378E-02
233	2.12749397E-01	9.13087539E-02
234	2.14324436E-01	9.15916609E-02
235	2.15870936E-01	9.18599239E-02
236	2.17389627E-01	9.21142784E-02
237	2.18880141E-01	9.23550281E-02
238	2.20344937E-01	9.25827466E-02
239	2.21787044E-01	9.27979264E-02
240	2.23202518E-01	9.30010493E-02
241	2.24594133E-01	9.31925865E-02
242	2.2596256E-01	9.33729982E-02
243	2.27309384E-01	9.35427344E-02
244	2.28633745E-01	9.37022342E-02
245	2.29935721E-01	9.38519262E-02
246	2.31222093E-01	9.39922289E-02
247	2.32484651E-01	9.41233549E-02
248	2.33733079E-01	9.42462869E-02
249	2.34958460E-01	9.43609827E-02
250	2.36168873E-01	9.44675490E-02

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LOWEST ENERGY STATE IS 1.194 RYDBERGS. RADIAL WAVE
R(R) AND PSI(R) WITH R IN 1/100 BOHR UNITS

R	R(R)	PSI(R)
251	2.37362717E-01	9.45668193E-02
252	2.38540670E-01	9.46599960E-02
253	2.39707400E-01	9.47444270E-02
254	2.40851566E-01	9.48234510E-02
255	2.41985312E-01	9.48963970E-02
256	2.43106777E-01	9.49635949E-02
257	2.44215036E-01	9.50253252E-02
258	2.45311353E-01	9.50819196E-02
259	2.46396182E-01	9.51336610E-02
260	2.47470164E-01	9.51808533E-02
261	2.48533898E-01	9.52233711E-02
262	2.49587918E-01	9.52625641E-02
263	2.50632815E-01	9.52976494E-02
264	2.51666912E-01	9.53292155E-02
265	2.52697396E-01	9.53575080E-02
266	2.53718142E-01	9.53822760E-02
267	2.54731896E-01	9.54052006E-02
268	2.55739127E-01	9.54255047E-02
269	2.56740352E-01	9.54440512E-02
270	2.57736266E-01	9.54605782E-02
271	2.58726716E-01	9.54751112E-02
272	2.59712769E-01	9.54882635E-02
273	2.60694674E-01	9.54992554E-02
274	2.61672239E-01	9.55091047E-02
275	2.62647730E-01	9.55180328E-02
276	2.63619824E-01	9.55261442E-02
277	2.64589403E-01	9.55334602E-02
278	2.65556915E-01	9.55399700E-02
279	2.66522740E-01	9.55456786E-02
280	2.67487254E-01	9.55505311E-02
281	2.68450318E-01	9.55544988E-02
282	2.69413734E-01	9.55576802E-02
283	2.70376493E-01	9.55600939E-02
284	2.71339237E-01	9.55617419E-02
285	2.72302458E-01	9.55626472E-02
286	2.73266346E-01	9.55628767E-02
287	2.74231241E-01	9.55624309E-02
288	2.75197435E-01	9.55615466E-02
289	2.76165209E-01	9.55602296E-02
290	2.77134834E-01	9.55584735E-02
291	2.78106571E-01	9.55563026E-02
292	2.79080672E-01	9.55537570E-02
293	2.80057300E-01	9.55508273E-02
294	2.81036926E-01	9.55475913E-02
295	2.82019536E-01	9.55439984E-02
296	2.83005421E-01	9.55400939E-02
297	2.83994788E-01	9.55362114E-02
298	2.84987333E-01	9.55333501E-02
299	2.85984741E-01	9.55304707E-02
300	2.86985569E-01	9.55281897E-02

TABLE VII

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LOWEST ENERGY STATE IS 1.194 RYDBERGS. RADIAL WAVE
R(R) AND PSI(R) WITH R IN 1/100 BCHR UNITS

R	R(R)	PSI(R)
301	2.87990728E-01	9.567779227E-02
302	2.890000016E-01	9.56953696E-02
303	2.90013720E-01	9.57140991E-02
304	2.91032005E-01	9.57342123E-02
305	2.92055035E-01	9.57557492E-02
306	2.93082975E-01	9.57787499E-02
307	2.94115998E-01	9.58032556E-02
308	2.95154241E-01	9.58292999E-02
309	2.96197896E-01	9.58569243E-02
310	2.97247119E-01	9.58861675E-02
311	2.98302074E-01	9.59170657E-02
312	2.99362926E-01	9.59499655E-02
313	3.00429840E-01	9.59833974E-02
314	3.01502980E-01	9.60200057E-02
315	3.02582510E-01	9.60579399E-02
316	3.03668597E-01	9.60976572E-02
317	3.04761404E-01	9.61392244E-02
318	3.05861098E-01	9.61822735E-02
319	3.06967843E-01	9.62269163E-02
320	3.08081904E-01	9.62735568E-02
321	3.09203148E-01	9.63224969E-02
322	3.10332039E-01	9.63736409E-02
323	3.11468644E-01	9.64269930E-02
324	3.12613130E-01	9.64835535E-02
325	3.13765661E-01	9.65433280E-02
326	3.14926405E-01	9.66065191E-02
327	3.16095528E-01	9.66735999E-02
328	3.17273198E-01	9.67446822E-02
329	3.18459581E-01	9.67796225E-02
330	3.19654846E-01	9.68695104E-02
331	3.20859139E-01	9.69363301E-02
332	3.22072690E-01	9.70099846E-02
333	3.23295606E-01	9.70895767E-02
334	3.24528807E-01	9.71644094E-02
335	3.25777027E-01	9.72449568E-02
336	3.27022357E-01	9.73280825E-02
337	3.28284507E-01	9.74133002E-02
338	3.29556890E-01	9.75020394E-02
339	3.30832676E-01	9.75928349E-02
340	3.32113305E-01	9.76861876E-02
341	3.33409714E-01	9.77821543E-02
342	3.34752178E-01	9.78807522E-02
343	3.36078220E-01	9.79822003E-02
344	3.37415679E-01	9.80885951E-02
345	3.38764449E-01	9.81926061E-02
346	3.40124222E-01	9.83002005E-02
347	3.41497139E-01	9.84141610E-02
348	3.42881131E-01	9.85291140E-02
349	3.44277632E-01	9.86468859E-02
350	3.45686260E-01	9.87675029E-02

TABLE VII

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LOWEST ENERGY STATE IS 1.194 RYDBERGS. RADIAL WAVE
R(R) AND PSI(R) WITH R IN 1/100 BOHR UNITS

R	R(R)	PSI(R)
351	3.47107379E-01	9.83909910E-02
352	3.48541165E-01	9.90173764E-02
353	3.49987797E-01	9.91466847E-02
354	3.51447454E-01	9.92729418E-02
355	3.52920315E-01	9.94141733E-02
356	3.54406561E-01	9.95524049E-02
357	3.55906373E-01	9.96933661E-02
358	3.57419972E-01	9.98379697E-02
359	3.58947420E-01	9.99855393E-02
360	3.604899021E-01	1.00145839E-01
361	3.62044920E-01	1.00289451E-01
362	3.63615300E-01	1.00446621E-01
363	3.65200034E-01	1.00606156E-01
364	3.66800024E-01	1.00769299E-01
365	3.68415191E-01	1.00935566E-01
366	3.70045364E-01	1.01105291E-01
367	3.71690095E-01	1.01278189E-01
368	3.73352155E-01	1.01454390E-01
369	3.75029154E-01	1.01633917E-01
370	3.76722146E-01	1.01816796E-01
371	3.78431323E-01	1.02003052E-01
372	3.80156878E-01	1.02192709E-01
373	3.81899007E-01	1.02385797E-01
374	3.83657997E-01	1.02582339E-01
375	3.85433777E-01	1.02782273E-01
376	3.87226805E-01	1.02985525E-01
377	3.89037201E-01	1.03192292E-01
378	3.90865163E-01	1.03403402E-01
379	3.92710891E-01	1.03617649E-01
380	3.94574539E-01	1.03835541E-01
381	3.96456643E-01	1.04056814E-01
382	3.98356711E-01	1.04281863E-01
383	4.00275546E-01	1.04510587E-01
384	4.02213175E-01	1.04743301E-01
385	4.04169803E-01	1.04979917E-01
386	4.06145647E-01	1.05221008E-01
387	4.08140913E-01	1.05466274E-01
388	4.10155381E-01	1.05715026E-01
389	4.12190569E-01	1.05968158E-01
390	4.14245399E-01	1.06226766E-01
391	4.16320427E-01	1.06487582E-01
392	4.18416029E-01	1.06753830E-01
393	4.20532428E-01	1.07025707E-01
394	4.22669700E-01	1.07297657E-01
395	4.24828140E-01	1.07575514E-01
396	4.27007970E-01	1.07853029E-01
397	4.29209412E-01	1.08131132E-01
398	4.31433271E-01	1.08400017E-01
399	4.33679080E-01	1.08669124E-01
400	4.35945753E-01	1.08938643E-01

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LOWEST ENERGY STATE IS 1.194 RYDBERGS. RADIAL WAVE
R(R) AND PSI(R) WITH R IN 1/100 BOHR UNITS

R	R(R)	PSI(R)
401	4.38235964E-01	1.09285777E-01
402	4.40548948E-01	1.09589290E-01
403	4.42884939E-01	1.09897007E-01
404	4.45244176E-01	1.10208955E-01
405	4.47626899E-01	1.10525160E-01
406	4.50033348E-01	1.10845652E-01
407	4.52463766E-01	1.11170458E-01
408	4.54918398E-01	1.11499607E-01
409	4.57397492E-01	1.11833129E-01
410	4.59901295E-01	1.12171047E-01
411	4.62430057E-01	1.12513396E-01
412	4.64984033E-01	1.12860202E-01
413	4.67563475E-01	1.13211495E-01
414	4.70168640E-01	1.13567304E-01
415	4.72799784E-01	1.13927659E-01
416	4.75457176E-01	1.14292590E-01
417	4.78141063E-01	1.14662127E-01
418	4.80851720E-01	1.15036199E-01
419	4.83589427E-01	1.15414513E-01
420	4.86354499E-01	1.15797667E-01
421	4.89147007E-01	1.16185693E-01
422	4.91967454E-01	1.16577996E-01
423	4.94815295E-01	1.16977774E-01
424	4.97692938E-01	1.17385041E-01
425	5.00593574E-01	1.17787900E-01
426	5.03533174E-01	1.18200275E-01
427	5.06497023E-01	1.18617570E-01
428	5.09490409E-01	1.19039815E-01
429	5.12513621E-01	1.19467045E-01
430	5.15566951E-01	1.19899391E-01
431	5.18650694E-01	1.20336588E-01
432	5.21765147E-01	1.20778969E-01
433	5.24910609E-01	1.21226468E-01
434	5.28087382E-01	1.21679120E-01
435	5.31295771E-01	1.22136959E-01
436	5.34536083E-01	1.22600019E-01
437	5.37809629E-01	1.23068336E-01
438	5.41113721E-01	1.23541946E-01
439	5.44451675E-01	1.24020883E-01
440	5.47822809E-01	1.24505184E-01
441	5.51227444E-01	1.24994985E-01
442	5.54665903E-01	1.25490002E-01
443	5.58138514E-01	1.25990655E-01
444	5.61645607E-01	1.26496758E-01
445	5.65187513E-01	1.27008450E-01
446	5.68764568E-01	1.27525688E-01
447	5.72377112E-01	1.28048571E-01
448	5.76025485E-01	1.28577117E-01
449	5.79711003E-01	1.29111366E-01
450	5.83431103E-01	1.29651356E-01

TABLE VII

GOLD

LOWEST ENERGY STATE IS 1.194 RYDBERGS. RADIAL WAVE
R(R) AND PSI(R) WITH R IN 1/100 BOHR UNITS

R	R(R)	PSI(R)
451	5.87189045E-01	1.30197123E-01
452	5.90984215E-01	1.30748720E-01
453	5.94816970E-01	1.31306174E-01
454	5.98687670E-01	1.31862531E-01
455	6.02596679E-01	1.32438831E-01
456	6.06544363E-01	1.33014115E-01
457	6.10531093E-01	1.33595426E-01
458	6.14557253E-01	1.34182806E-01
459	6.18623206E-01	1.34776298E-01
460	6.22729339E-01	1.35375943E-01
461	6.26876036E-01	1.35981787E-01
462	6.31063686E-01	1.36593271E-01
463	6.35292631E-01	1.37212242E-01
464	6.39566341E-01	1.37836943E-01
465	6.43876288E-01	1.38468010E-01
466	6.48231702E-01	1.39103351E-01
467	6.52630065E-01	1.39742947E-01
468	6.57071787E-01	1.40399954E-01
469	6.61557332E-01	1.41056990E-01
470	6.66086968E-01	1.41720637E-01
471	6.70661267E-01	1.42390927E-01
472	6.75280606E-01	1.43067925E-01
473	6.79945415E-01	1.43751673E-01
474	6.84656128E-01	1.44442221E-01
475	6.89413183E-01	1.45139961E-01
476	6.94217024E-01	1.45843913E-01
477	6.99068096E-01	1.46555156E-01
478	7.03966352E-01	1.47273400E-01
479	7.08913746E-01	1.47998694E-01
480	7.13909237E-01	1.48731091E-01
481	7.18953792E-01	1.49470643E-01
482	7.24047878E-01	1.50217402E-01
483	7.29191967E-01	1.50971439E-01
484	7.34386528E-01	1.51732756E-01
485	7.39632073E-01	1.52501459E-01
486	7.44929059E-01	1.53277594E-01
487	7.50277927E-01	1.54061163E-01
488	7.55679355E-01	1.54852327E-01
489	7.61133662E-01	1.55651056E-01
490	7.66641416E-01	1.56457432E-01
491	7.72203126E-01	1.57271513E-01
492	7.77819310E-01	1.58093356E-01
493	7.83490480E-01	1.58923020E-01
494	7.89217126E-01	1.59760564E-01
495	7.94999935E-01	1.60606047E-01
496	8.00833927E-01	1.61459530E-01
497	8.06735573E-01	1.62321074E-01
498	8.12689877E-01	1.63190739E-01
499	8.18702246E-01	1.64068586E-01
500	8.24773400E-01	1.64954680E-01

TABLE VII

GOLD

LOWEST ENERGY STATE IS .1.194 RYDBERGS. RADIAL WAVE
R(R) AND PSI(R) WITH P IN 1/100 BOHR UNITS

R	R(R)	PSI(R)
501	8.30903902E-01	1.65649082E-01
502	8.37094323E-01	1.66751857E-01
503	8.43345235E-01	1.67663069E-01
504	8.49657217E-01	1.68582781E-01
505	8.56030856E-01	1.69511061E-01
506	8.62466743E-01	1.70447973E-01
507	8.68965474E-01	1.71393585E-01
508	8.75527653E-01	1.72347963E-01
509	8.82153889E-01	1.73311177E-01
510	8.88844796E-01	1.74283293E-01
511	8.95600996E-01	1.75264383E-01
512	9.02423115E-01	1.76254515E-01
513	9.09311796E-01	1.77253759E-01
514	9.16267650E-01	1.78262189E-01
515	9.23291352E-01	1.79279274E-01
516	9.30383544E-01	1.80306888E-01
517	9.37544886E-01	1.81343305E-01
518	9.44776040E-01	1.82389197E-01
519	9.52077630E-01	1.83444640E-01
520	9.59450488E-01	1.84509709E-01
521	9.66895144E-01	1.85584481E-01
522	9.74412342E-01	1.86669031E-01
523	9.82002781E-01	1.87763438E-01
524	9.89667166E-01	1.88867780E-01
525	9.97406211E-01	1.89982135E-01
526	1.00522064E+00	1.91106595E-01
527	1.01311117E+00	1.92241202E-01
528	1.02107854E+00	1.93386087E-01
529	1.02912349E+00	1.94541303E-01
530	1.03724678E+00	1.95706940E-01
531	1.04544916E+00	1.96883080E-01
532	1.05373139E+00	1.98069809E-01
533	1.06209424E+00	1.99267212E-01
534	1.07053950E+00	2.00475374E-01
535	1.07906495E+00	2.01694382E-01
536	1.08767438E+00	2.02924325E-01
537	1.09636761E+00	2.04165290E-01
538	1.10514543E+00	2.05417367E-01
539	1.11400868E+00	2.06682064E-01
540	1.12295817E+00	2.07955217E-01
541	1.13199475E+00	2.09241174E-01
542	1.14111926E+00	2.10538603E-01
543	1.15033254E+00	2.11847614E-01
544	1.15963554E+00	2.13168285E-01
545	1.16902891E+00	2.14500717E-01
546	1.17851373E+00	2.15845606E-01
547	1.18809093E+00	2.17201250E-01
548	1.19777611E+00	2.18569547E-01
549	1.20752547E+00	2.19949952E-01
550	1.21738482E+00	2.21342695E-01

TABLE VII

GOLD

LOWEST ENERGY STATE IS 1.194 RYDBERGS. RADIAL WAVE
R(R) AND PSI(R) WITH R IN 1/100 BOHR UNITS

R	R(R)	PSI(R)
551	1.22734009E+00	2.22747748E-01
552	1.23739221E+00	2.24145255E-01
553	1.24754212E+00	2.25595319E-01
554	1.25779077E+00	2.27038045E-01
555	1.26813912E+00	2.28493553E-01
556	1.27858816E+00	2.29961899E-01
557	1.28913885E+00	2.31443240E-01
558	1.29979218E+00	2.32937667E-01
559	1.31054917E+00	2.34445289E-01
560	1.32141081E+00	2.35966216E-01
561	1.33237813E+00	2.37500559E-01
562	1.34345217E+00	2.39048428E-01
563	1.35463395E+00	2.40609938E-01
564	1.36592454E+00	2.42185203E-01
565	1.37732500E+00	2.43774337E-01
566	1.38883640E+00	2.45377456E-01
567	1.40045982E+00	2.46994678E-01
568	1.41219637E+00	2.48626121E-01
569	1.42404714E+00	2.50271905E-01
570	1.43601325E+00	2.51932150E-01
571	1.44809584E+00	2.53606977E-01
572	1.46029604E+00	2.55296511E-01
573	1.47261501E+00	2.57000874E-01
574	1.48505390E+00	2.58720192E-01
575	1.49761390E+00	2.60454591E-01
576	1.51029619E+00	2.62204199E-01
577	1.52310197E+00	2.63969145E-01
578	1.53603245E+00	2.65749553E-01
579	1.54908935E+00	2.67545570E-01
580	1.56227241E+00	2.69357312E-01
581	1.57558438E+00	2.71184920E-01
582	1.58902602E+00	2.73028526E-01
583	1.60259961E+00	2.74888326E-01
584	1.61630342E+00	2.76764285E-01
585	1.63014177E+00	2.78656712E-01
586	1.64411495E+00	2.80565692E-01
587	1.65822431E+00	2.82491364E-01
588	1.67247117E+00	2.84433873E-01
589	1.68685690E+00	2.86393362E-01
590	1.70137286E+00	2.88369975E-01
591	1.71605042E+00	2.90363861E-01
592	1.73086099E+00	2.92375167E-01
593	1.74581597E+00	2.94404043E-01
594	1.76091679E+00	2.96450639E-01
595	1.77616489E+00	2.98515107E-01
596	1.79156171E+00	3.00597603E-01
597	1.80710873E+00	3.02698279E-01
598	1.82280742E+00	3.04817295E-01
599	1.83865929E+00	3.06954806E-01
600	1.85466534E+00	3.09110974E-01

TABLE VII

GOLD

LOWEST ENERGY STATE IS 1.194 RYDBERGS. RADIAL WAVE
R(R) AND PSI(R) WITH R IN 1/100 BOHR UNITS

R	R(R)	PSI(R)
601	1.87082861E+00	3.11285558E-01
602	1.88714913E+00	3.13479923E-01
603	1.90362897E+00	3.15693030E-01
604	1.92026970E+00	3.17925448E-01
605	1.93707292E+00	3.20177342E-01
606	1.95404022E+00	3.22448881E-01
607	1.97117323E+00	3.24740236E-01
608	1.98847359E+00	3.27051578E-01
609	2.00594297E+00	3.29383082E-01
610	2.02358302E+00	3.31734922E-01
611	2.04139545E+00	3.34107273E-01
612	2.05938195E+00	3.36500319E-01
613	2.07754427E+00	3.38914236E-01
614	2.09588412E+00	3.41340206E-01
615	2.11440329E+00	3.43805413E-01
616	2.13310354E+00	3.46298043E-01
617	2.15198668E+00	3.48782228E-01
618	2.17105451E+00	3.51303312E-01
619	2.19030987E+00	3.53846344E-01
620	2.20975169E+00	3.56411561E-01
621	2.22933246E+00	3.58999132E-01
622	2.24920976E+00	3.61609288E-01
623	2.26922895E+00	3.64242207E-01
624	2.28944411E+00	3.66899302E-01
625	2.30985723E+00	3.69577156E-01
626	2.33047023E+00	3.72279589E-01
627	2.35128511E+00	3.75000560E-01
628	2.37230339E+00	3.77755396E-01
629	2.39352859E+00	3.80529188E-01
630	2.41496126E+00	3.83322718E-01
631	2.43660398E+00	3.86149601E-01
632	2.45845883E+00	3.88999665E-01
633	2.48052793E+00	3.91968552E-01
634	2.50281741E+00	3.94947655E-01
635	2.52531744E+00	3.97627785E-01
636	2.54800421E+00	4.00635562E-01
637	2.57098933E+00	4.03609079E-01
638	2.59416268E+00	4.06608563E-01
639	2.61756232E+00	4.09634244E-01
640	2.64119256E+00	4.12696354E-01
641	2.66505445E+00	4.15765126E-01
642	2.68915063E+00	4.18870796E-01
643	2.71348317E+00	4.22000360E-01
644	2.73805480E+00	4.25163789E-01
645	2.76286779E+00	4.28351594E-01
646	2.78792453E+00	4.31567264E-01
647	2.81322747E+00	4.34811047E-01
648	2.83877909E+00	4.38083192E-01
649	2.86458135E+00	4.41383952E-01
650	2.89063827E+00	4.44713581E-01

TABLE VII

GOLD

LOWEST ENERGY STATE IS 1.194 RYDBERGS. RADIAL WAVE
R(R) AND PSI(R) WITH R IN 1/100 BOHR UNITS

R	R(R)	PSI(R)
651	2.9162509CE+CO	4.48072334E-01
652	2.94352219E+CO	4.51460459E-01
653	2.97035465E+CO	4.54878200E-01
654	2.99745079E+CO	4.58325809E-01
655	3.02481316E+CO	4.61803536E-01
656	3.05244434E+CO	4.65311637E-01
657	3.08034691E+CO	4.68850367E-01
658	3.10852351E+CO	4.72419986E-01
659	3.13697678E+CO	4.76020756E-01
660	3.16570940E+CO	4.79652940E-01
661	3.19472408E+CO	4.83316805E-01
662	3.22402355E+CO	4.87012620E-01
663	3.25361056E+CO	4.90740657E-01
664	3.28348790E+CO	4.94501190E-01
665	3.31365839E+CO	4.98294435E-01
666	3.34412487E+CO	5.02120932E-01
667	3.37489022E+CO	5.05992054E-01
668	3.40595735E+CO	5.09973852E-01
669	3.43732914E+CO	5.13801068E-01
670	3.46900861E+CO	5.17762479E-01
671	3.50099872E+CO	5.21758379E-01
672	3.53330251E+CO	5.25789906E-01
673	3.56592301E+CO	5.29854830E-01
674	3.59886371E+CO	5.33955930E-01
675	3.63212659E+CO	5.38092281E-01
676	3.66571579E+CO	5.42265649E-01
677	3.69967429E+CO	5.46474785E-01
678	3.73388524E+CO	5.50720357E-01
679	3.76847186E+CO	5.55003220E-01
680	3.80339745E+CO	5.59323154E-01
681	3.83866529E+CO	5.63670659E-01
682	3.87427873E+CO	5.68076080E-01
683	3.91024115E+CO	5.72509685E-01
684	3.94655595E+CO	5.76981864E-01
685	3.98322657E+CO	5.81492230E-01
686	4.02025649E+CO	5.86043220E-01
687	4.05764922E+CO	5.90633074E-01
688	4.09540830E+CO	5.95262835E-01
689	4.13353733E+CO	5.99932294E-01
690	4.17203991E+CO	6.04643465E-01
691	4.21091971E+CO	6.09395037E-01
692	4.25012041E+CO	6.14187920E-01
693	4.289922574E+CO	6.19022474E-01
694	4.32985948E+CO	6.23899060E-01
695	4.37028542E+CO	6.28811804E-01
696	4.41110741E+CO	6.33779900E-01
697	4.45232932E+CO	6.38792469E-01
698	4.49395510E+CO	6.43833109E-01
699	4.53593868E+CO	6.48925419E-01
700	4.57843408E+CO	6.54062011E-01

TABLE VII

GOLD

LOWEST LNERGY STATE IS 1.194 RYDBERGS. RADIAL WAVE
R(R) AND PSI(R) WITH R IN 1/100 BOHR UNITS

R	R(R)	PSI(R)
701	4.62129532E+00	6.59243270E-01
702	4.66457650E+00	6.64469583E-01
703	4.70322917E+00	6.69741357E-01
704	4.75241520E+00	6.75058977E-01
705	4.79692109E+00	6.80422849E-01
706	4.84192365E+00	6.85833378E-01
707	4.88742717E+00	6.91290972E-01
708	4.93331600E+00	6.96796045E-01
709	4.97965450E+00	7.02349017E-01
710	5.02644711E+00	7.07950297E-01
711	5.07369829E+00	7.13600721E-01
712	5.12141254E+00	7.19299514E-01
713	5.16959443E+00	7.25048307E-01
714	5.21824856E+00	7.30847137E-01
715	5.26737958E+00	7.36696444E-01
716	5.31699218E+00	7.42596674E-01
717	5.36709112E+00	7.48548273E-01
718	5.41768117E+00	7.54551696E-01
719	5.46876719E+00	7.60607398E-01
720	5.52035406E+00	7.66715841E-01
721	5.57244467E+00	7.72877491E-01
722	5.62505014E+00	7.79092817E-01
723	5.67816938E+00	7.85362293E-01
724	5.73180952E+00	7.91686399E-01
725	5.78597570E+00	7.98065614E-01
726	5.84067312E+00	8.04500042E-01
727	5.89590701E+00	8.10991333E-01
728	5.95168267E+00	8.17538829E-01
729	6.00800546E+00	8.24143410E-01
730	6.06488077E+00	8.30830559E-01
731	6.12231407E+00	8.37525565E-01
732	6.18031087E+00	8.44330476E-01
733	6.23897674E+00	8.51142302E-01
734	6.29901750E+00	8.58040504E-01
735	6.35777824E+00	8.64992819E-01
736	6.41804529E+00	8.72017023E-01
737	6.47894425E+00	8.79096913E-01
738	6.54044097E+00	8.86258619E-01
739	6.60254138E+00	8.93442677E-01
740	6.66525143E+00	9.00709655E-01
741	6.72857720E+00	9.08040103E-01
742	6.79252474E+00	9.15474601E-01
743	6.85710022E+00	9.22893703E-01
744	6.92230935E+00	9.30417991E-01
745	6.98815993E+00	9.38008044E-01
746	7.05465679E+00	9.45664449E-01
747	7.12180685E+00	9.53387797E-01
748	7.18961657E+00	9.61178686E-01
749	7.25809249E+00	9.69037716E-01
750	7.32724123E+00	9.76965497E-01

TABLE VII

GOLD

LOWEST ENERGY STATE IS 1.194 RYDBERGS. RADIAL WAVE
R(R) AND PSI(R) WITH R IN 1/100 BOHR UNITS

R	R(R)	PSI(R)
751	7.39706945E+00	9.84962643E-01
752	7.46758398E+00	9.93029771E-01
753	7.53879133E+00	1.00116751E+00
754	7.61069369E+00	1.00957448E+00
755	7.68531289E+00	1.01765734E+00
756	7.75664094E+00	1.02601071E+00
757	7.83068793E+00	1.03443724E+00
758	7.90546702E+00	1.04293760E+00
759	7.98097944E+00	1.05151244E+00
760	8.05723448E+00	1.06016243E+00
761	8.13423953E+00	1.06888824E+00
762	8.21200202E+00	1.07776905E+00
763	8.29052949E+00	1.08665700E+00
764	8.36982953E+00	1.09555274E+00
765	8.44990093E+00	1.10456338E+00
766	8.53077813E+00	1.11367861E+00
767	8.61244227E+00	1.12289783E+00
768	8.69491017E+00	1.13221497E+00
769	8.77813990E+00	1.14165071E+00
770	8.86220971E+00	1.15109466E+00
771	8.94721467E+00	1.16064690E+00
772	9.03292003E+00	1.17030751E+00
773	9.11958843E+00	1.18007656E+00
774	9.20704950E+00	1.18995412E+00
775	9.29537199E+00	1.19994028E+00
776	9.38456446E+00	1.20993510E+00
777	9.47463557E+00	1.21994868E+00
778	9.56559409E+00	1.22995108E+00
779	9.65744333E+00	1.23992723E+00
780	9.75020872E+00	1.24990026E+00
781	9.84382279E+00	1.25987020E+00
782	9.93842012E+00	1.26983703E+00
783	1.00340099E+01	1.27979953E+00
784	1.01304315E+01	1.28975875E+00
785	1.02279042E+01	1.29971477E+00
786	1.03262876E+01	1.30966750E+00
787	1.04256412E+01	1.31961693E+00
788	1.05259746E+01	1.32956308E+00
789	1.06273297E+01	1.33950593E+00
790	1.07296203E+01	1.34944547E+00
791	1.08328952E+01	1.35938179E+00
792	1.09373040E+01	1.36931490E+00
793	1.10426895E+01	1.37924491E+00
794	1.11491066E+01	1.38917182E+00
795	1.12565733E+01	1.39909573E+00
796	1.13651109E+01	1.40901664E+00
797	1.14747149E+01	1.41893455E+00
798	1.15854010E+01	1.42884946E+00
799	1.16971801E+01	1.43876137E+00
800	1.18100630E+01	1.44867028E+00

TABLE VII

GOLD

LOWEST ENERGY STATE IS 1.194 RYDBERGS. RADIAL WAVE
R(R) AND PSI(R) WITH R IN 1/100 BOHR UNITS

R	R(R)	PSI(R)
801	1.19240608E+01	1.48864679E+00
802	1.20391845E+01	1.50114521E+00
803	1.21554456E+01	1.51375412E+00
804	1.22728552E+01	1.52647453E+00
805	1.23914250E+01	1.53930745E+00
806	1.25111664E+01	1.55225389E+00
807	1.26320911E+01	1.56531489E+00
808	1.27542111E+01	1.57849148E+00
809	1.28775383E+01	1.59178471E+00
810	1.30020846E+01	1.60519563E+00
811	1.31278624E+01	1.61872533E+00
812	1.32548859E+01	1.63237487E+00
813	1.33831616E+01	1.64614534E+00
814	1.35127080E+01	1.66003783E+00
815	1.36435357E+01	1.67405347E+00
816	1.37756578E+01	1.68821933E+00
817	1.39090369E+01	1.70245862E+00
818	1.40433364E+01	1.71685041E+00
819	1.41799193E+01	1.73136988E+00
820	1.43173400E+01	1.74601817E+00
821	1.44561390E+01	1.76079647E+00
822	1.45963029E+01	1.77570595E+00
823	1.47379540E+01	1.79074731E+00
824	1.48802074E+01	1.80592325E+00
825	1.50251764E+01	1.82123349E+00
826	1.51709748E+01	1.83667975E+00
827	1.53182173E+01	1.85226328E+00
828	1.54669184E+01	1.86798531E+00
829	1.56170926E+01	1.88384712E+00
830	1.57687548E+01	1.89984997E+00

TIME, 0 MINUTES AND 59 SECONDS

TABLE VIII

GOLD

LOWEST ENERGY STATE IS 1.194 RYDBERGS. RADIAL WAVE
FUNCTIONS $R(r)$ AND $\Psi(r)\Psi(r)^*$ WITH r IN 1/100
BOHR UNITS.

R	$\Psi(r)\Psi(r)^*$
1	5.93189234E-01
2	1.26805980E+00
3	9.31935645E-01
4	2.17757251E-01
5	1.30323549E-03
6	6.66528726E-02
7	1.80637782E-01
8	2.29520372E-01
9	2.29074420E-01
10	1.74401300E-01
11	1.06943654E-01
12	4.96832492E-02
13	1.37235222E-02
14	3.25199885E-04
15	4.76931949E-03
16	1.98961260E-02
17	3.86570303E-02
18	5.55423358E-02
19	6.71471257E-02
20	7.20249897E-02
21	7.73437908E-02
22	6.73455041E-02
23	5.27855353E-02
24	4.05639775E-02
25	2.83876116E-02
26	1.76030287E-02
27	9.11333672E-03
28	3.47957028E-03
29	4.73897770E-04
30	1.62466085E-04
31	1.99928293E-03
32	5.41754579E-03
33	9.51020797E-03
34	1.45931127E-02
35	1.92523769E-02
36	2.33730602E-02
37	2.66534051E-02
38	2.89064634E-02
39	3.00523253E-02
40	3.01042771E-02
41	2.91502886E-02
42	2.73341563E-02
43	2.48359549E-02
44	2.18543338E-02
45	1.85910878E-02
46	1.52335363E-02
47	1.19698880E-02
48	8.93252076E-03
49	6.24397008E-03
50	3.99027210E-03

TABLE VIII

GOLD

LOWEST ENERGY STATE IS 1.194 RYDBERGS. RADIAL WAVE
FUNCTIONS $R(r)$ AND $\Psi(r)\Psi(r)^*$ WITH r IN $1/100$
BOHR UNITS.

R	$\Psi(r)\Psi(r)^*$
51	2.32627863E-03
52	9.77523835E-04
53	2.43235664E-04
54	1.13352901E-07
55	2.06535388E-04
56	8.06212938E-04
57	1.73555722E-03
58	2.92258203E-03
59	4.29401250E-03
60	5.77791422E-03
61	7.30599824E-03
62	8.21558567E-03
63	1.02512446E-02
64	1.15658299E-02
65	1.27210707E-02
66	1.36877606E-02
67	1.44456088E-02
68	1.49828150E-02
69	1.52954256E-02
70	1.53865301E-02
71	1.52653490E-02
72	1.49452593E-02
73	1.44478016E-02
74	1.37916924E-02
75	1.30018862E-02
76	1.21036934E-02
77	1.11229776E-02
78	1.00854430E-02
79	9.01601628E-03
80	7.93932759E-03
81	6.87428876E-03
82	5.84376645E-03
83	4.86434433E-03
84	3.95116835E-03
85	3.11636597E-03
86	2.37153236E-03
87	1.72277342E-03
88	1.17579745E-03
89	7.33546478E-04
90	3.96859068E-04
91	1.64656768E-04
92	3.41470704E-05
93	1.03645815E-06
94	5.97478278E-05
95	2.03637533E-04
96	4.25206442E-04
97	7.16305717E-04
98	1.06832749E-03
99	1.47238524E-03
100	1.91947812E-03

TABLE VIII

GOLD

LOWEST ENERGY STATE IS 1.194 RYDBERGS. RADIAL WAVE
FUNCTIONS $R(r)$ AND $\Psi(r)\Psi(r)^*$ WITH r IN 1/100
BOHR UNITS.

R	$\Psi(r)\Psi(r)^*$
101	2.40063947E-03
102	2.90706867E-03
103	3.43024630E-03
104	3.96203243E-03
105	4.49474863E-03
106	5.02124463E-03
107	5.53494933E-03
108	6.0290901E-03
109	6.50081192E-03
110	6.94300192E-03
111	7.35248068E-03
112	7.72590192E-03
113	8.06055658E-03
114	8.35435151E-03
115	8.60578232E-03
116	8.81400143E-03
117	8.97928242E-03
118	9.09908149E-03
119	9.17649699E-03
120	9.21172762E-03
121	9.20523014E-03
122	9.16067710E-03
123	9.07781510E-03
124	8.95942410E-03
125	8.80777809E-03
126	8.62530751E-03
127	8.41456358E-03
128	8.17318430E-03
129	7.91936579E-03
130	7.63932842E-03
131	7.34229556E-03
132	7.03046714E-03
133	6.70649877E-03
134	6.37298275E-03
135	6.03243149E-03
136	5.68726308E-03
137	5.33978923E-03
138	4.99220520E-03
139	4.64658147E-03
140	4.30435767E-03
141	3.96333782E-03
142	3.64018731E-03
143	3.32043128E-03
144	3.01095423E-03
145	2.71300086E-03
146	2.42767794E-03
147	2.15505704E-03
148	1.89867206E-03
149	1.65655352E-03
150	1.43017331E-03

TABLE VIII

GOLD

LOWEST ENERGY STATE IS 1.124 RYDBERGS. RADIAL WAVE
FUNCTIONS $R(r)$ AND $\Psi(r)\Psi(r)^*$ WITH r IN 1/100
BOHR UNITS.

R	$\Psi(r)\Psi(r)^*$
151	1.32031000E-02
152	1.02642450E-03
153	9.49672025E-04
154	6.39908271E-04
155	5.47195770E-04
156	4.21510301E-04
157	3.12747336E-04
158	2.20723466E-04
159	1.45207753E-04
160	8.58779769E-05
161	4.73767103E-05
162	1.42922604E-05
163	1.16937395E-06
164	2.51473579E-06
165	1.78022262E-05
166	4.44779264E-05
167	8.79648629E-05
168	1.41667494E-04
169	2.06975863E-04
170	2.83269639E-04
171	3.69921655E-04
172	4.66301370E-04
173	5.71777970E-04
174	6.85723237E-04
175	8.07514155E-04
176	9.36535239E-04
177	1.07218088E-03
178	1.21335682E-03
179	1.36098227E-03
180	1.51239116E-03
181	1.66953352E-03
182	1.82947652E-03
183	1.99290544E-03
184	2.15912443E-03
185	2.32755712E-03
186	2.49804715E-03
187	2.66935839E-03
188	2.84267529E-03
189	3.01610295E-03
190	3.18976713E-03
191	3.36331418E-03
192	3.53641032E-03
193	3.70874422E-03
194	3.88002107E-03
195	4.04996784E-03
196	4.21833007E-03
197	4.38487199E-03
198	4.54937597E-03
199	4.71154207E-03
200	4.87148741E-03

TABLE VIII

GOLD

LOWEST ENERGY STATE IS 1.124 RYDBERGS. RADIAL WAVE
FUNCTIONS $R(r)$ AND $\Psi(r)\Psi(r)^*$ WITH r IN $1/100$
BOHR UNITS.

R	$\Psi(r)\Psi(r)^*$
201	5.02874565E-03
202	5.18326636E-03
203	5.33491440E-03
204	5.48356936E-03
205	5.62912486E-03
206	5.77148798E-03
207	5.91057860E-03
208	6.04632878E-03
209	6.17858215E-03
210	6.30759329E-03
211	6.43330271E-03
212	6.55495838E-03
213	6.67337088E-03
214	6.78825713E-03
215	6.89961765E-03
216	7.00746054E-03
217	7.11130086E-03
218	7.21266020E-03
219	7.31096619E-03
220	7.40400010E-03
221	7.49245558E-03
222	7.58102071E-03
223	7.66539328E-03
224	7.74662641E-03
225	7.82417292E-03
226	7.89859114E-03
227	7.96994163E-03
228	8.03802874E-03
229	8.10359372E-03
230	8.16622762E-03
231	8.22595782E-03
232	8.28295440E-03
233	8.33729854E-03
234	8.38900322E-03
235	8.43835849E-03
236	8.48504028E-03
237	8.52945123E-03
238	8.57156497E-03
239	8.61145515E-03
240	8.64919518E-03
241	8.68435817E-03
242	8.71851680E-03
243	8.75024316E-03
244	8.78010869E-03
245	8.80816405E-03
246	8.83453907E-03
247	8.85924261E-03
248	8.88236257E-03
249	8.90396574E-03
250	8.92411782E-03

TABLE VIII

GOLD

LOWEST ENERGY STATE IS 1.194 RYDBERGS. RADIAL WAVE
FUNCTIONS $R(r)$ AND $\Psi(r)\Psi(r)^*$ WITH r IN $1/100$
BOHR UNITS.

251	8.94288332E-03
252	8.96032552E-03
253	8.97650645E-03
254	8.99148686E-03
255	9.00532617E-03
256	9.01838245E-03
257	9.02931243E-03
258	9.04057144E-03
259	9.05041345E-03
260	9.05939102E-03
261	9.06755532E-03
262	9.07495611E-03
263	9.08164179E-03
264	9.08765933E-03
265	9.09305433E-03
266	9.09737103E-03
267	9.10215230E-03
268	9.10593963E-03
269	9.10927325E-03
270	9.11219197E-03
271	9.11473337E-03
272	9.11693371E-03
273	9.11832801E-03
274	9.12045003E-03
275	9.12133223E-03
276	9.12300611E-03
277	9.12450016E-03
278	9.12484709E-03
279	9.12557279E-03
280	9.12620294E-03
281	9.12676404E-03
282	9.12728067E-03
283	9.12777635E-03
284	9.12827361E-03
285	9.12879394E-03
286	9.12935789E-03
287	9.12993503E-03
288	9.13069403E-03
289	9.13150260E-03
290	9.13242762E-03
291	9.13342507E-03
292	9.13469009E-03
293	9.13605702E-03
294	9.13759938E-03
295	9.13932290E-03
296	9.14126055E-03
297	9.14340259E-03
298	9.14576651E-03
299	9.14836212E-03
300	9.15119655E-03

TABLE VIII

GOLD

LOWEST ENERGY STATE IS 1.194 RYDBERGS. RADIAL WAVE
FUNCTIONS $R(r)$ AND $\Psi(r)\Psi(r)^*$ WITH r IN $1/100$
BOHR UNITS.

R	$\Psi(r)\Psi(r)^*$
301	9.15427637E-03
302	9.15760376E-03
303	9.16118877E-03
304	9.16503940E-03
305	9.16916351E-03
306	9.17356894E-03
307	9.17826340E-03
308	9.18325454E-03
309	9.18854294E-03
310	9.19415711E-03
311	9.20008347E-03
312	9.20633647E-03
313	9.21292233E-03
314	9.21995132E-03
315	9.22742779E-03
316	9.23534759E-03
317	9.24372754E-03
318	9.25251118E-03
319	9.26169359E-03
320	9.27128984E-03
321	9.28137949E-03
322	9.29192412E-03
323	9.30298729E-03
324	9.31450945E-03
325	9.32652050E-03
326	9.33906217E-03
327	9.35217441E-03
328	9.36588563E-03
329	9.38013695E-03
330	9.39496646E-03
331	9.41031029E-03
332	9.42621462E-03
333	9.44260361E-03
334	9.45950621E-03
335	9.47695563E-03
336	9.49499449E-03
337	9.51366474E-03
338	9.53290359E-03
339	9.55274259E-03
340	9.57322391E-03
341	9.59438613E-03
342	9.61626054E-03
343	9.63887474E-03
344	9.66220858E-03
345	9.68631787E-03
346	9.71123833E-03
347	9.73695347E-03
348	9.76347986E-03
349	9.79082099E-03
350	9.75501962E-03

TABLE VIII

GOLD

LOWEST ENERGY STATE IS 1.194 RYDBERGS. RADIAL WAVE
FUNCTIONS $R(r)$ AND $\Psi(r)\Psi(r)^*$ WITH r IN 1/100
BOHR UNITS.

R	$\Psi(r)\Psi(r)^*$
351	9.77942811E-03
352	9.80444082E-03
353	9.83006502E-03
354	9.85630829E-03
355	9.88317786E-03
356	9.91068132E-03
357	9.93882621E-03
358	9.96762020E-03
359	9.99707097E-03
360	1.00271865E-02
361	1.00579741E-02
362	1.00804422E-02
363	1.01215987E-02
364	1.01544516E-02
365	1.01900092E-02
366	1.02223798E-02
367	1.02527271E-02
368	1.02829932E-02
369	1.03224531E-02
370	1.03564660E-02
371	1.04046225E-02
372	1.04433498E-02
373	1.04828506E-02
374	1.05231240E-02
375	1.05642093E-02
376	1.06060858E-02
377	1.06487729E-02
378	1.06922801E-02
379	1.07366173E-02
380	1.07817941E-02
381	1.08278205E-02
382	1.08747066E-02
383	1.09224627E-02
384	1.09710920E-02
385	1.10206262E-02
386	1.10710547E-02
387	1.11223955E-02
388	1.11746594E-02
389	1.12278577E-02
390	1.12820015E-02
391	1.13371023E-02
392	1.13931716E-02
393	1.14502213E-02
394	1.15082633E-02
395	1.15673096E-02
396	1.16273726E-02
397	1.16884648E-02
398	1.17505988E-02
399	1.18137874E-02
400	1.18780437E-02

TABLE VIII

GOLD

LOWEST ENERGY STATE IS 1.194 RYDBERGS. RADIAL WAVE
FUNCTIONS $R(r)$ AND $\Psi(r)\Psi(r)^*$ WITH r IN 1/100
BOHR UNITS.

r	$\Psi(r)\Psi(r)^*$
401	1.19433810E-02
402	1.20098126E-02
403	1.20773522E-02
404	1.21460137E-02
405	1.22158110E-02
406	1.22867593E-02
407	1.23588702E-02
408	1.24321625E-02
409	1.25066488E-02
410	1.25823439E-02
411	1.26592643E-02
412	1.27374252E-02
413	1.28168426E-02
414	1.28975326E-02
415	1.29795116E-02
416	1.30627962E-02
417	1.31474033E-02
418	1.32333550E-02
419	1.33206540E-02
420	1.34093328E-02
421	1.34994043E-02
422	1.35909872E-02
423	1.36843727E-02
424	1.37783160E-02
425	1.38739293E-02
426	1.39713051E-02
427	1.40701279E-02
428	1.41704776E-02
429	1.42723747E-02
430	1.43758400E-02
431	1.44808944E-02
432	1.45875594E-02
433	1.46958567E-02
434	1.48058083E-02
435	1.49174367E-02
436	1.50307647E-02
437	1.51458154E-02
438	1.52626123E-02
439	1.53811794E-02
440	1.55015409E-02
441	1.56237213E-02
442	1.57477460E-02
443	1.58736402E-02
444	1.60014193E-02
445	1.61311413E-02
446	1.62628011E-02
447	1.63964365E-02
448	1.65320751E-02
449	1.66697448E-02
450	1.68094741E-02

TABLE VIII

GOLD

LOWEST ENERGY STATE IS 1.194 RYDBERGS. RADIAL WAVE
FUNCTIONS $R(r)$ AND $\Psi(r)\Psi(r)^*$ WITH r IN $1/100$
BOHR UNITS.

R	$\Psi(r)\Psi(r)^*$
451	1.69512920E-02
452	1.70952278E-02
453	1.72413114E-02
454	1.73895732E-02
455	1.75400439E-02
456	1.76927543E-02
457	1.78477372E-02
458	1.80050255E-02
459	1.81646504E-02
460	1.83266460E-02
461	1.84910463E-02
462	1.86578857E-02
463	1.88271994E-02
464	1.89990228E-02
465	1.91733922E-02
466	1.93503444E-02
467	1.95299168E-02
468	1.97121472E-02
469	1.98970743E-02
470	2.00847374E-02
471	2.02751761E-02
472	2.04684312E-02
473	2.06645436E-02
474	2.08635552E-02
475	2.10655086E-02
476	2.12704469E-02
477	2.14784139E-02
478	2.16894543E-02
479	2.19036135E-02
480	2.21209375E-02
481	2.23414731E-02
482	2.25652679E-02
483	2.27923702E-02
484	2.30228292E-02
485	2.32566948E-02
486	2.34940178E-02
487	2.37348492E-02
488	2.39792431E-02
489	2.42272511E-02
490	2.44789280E-02
491	2.47343287E-02
492	2.49935091E-02
493	2.52565262E-02
494	2.55234373E-02
495	2.57943025E-02
496	2.60691800E-02
497	2.63481309E-02
498	2.66312171E-02
499	2.69185010E-02
500	2.72100465E-02

TABLE VIII

GOLD

LOWEST ENERGY STATE IS 1.194 RYDBERGS. RADIAL WAVE
FUNCTIONS $R(r)$ AND $\Psi(r)\Psi(r)^*$ WITH r IN 1/100
BOHR UNITS.

r	$\Psi(r)\Psi(r)^*$
501	2.75059182E-02
502	2.78061819E-02
503	2.81109046E-02
504	2.84201541E-02
505	2.87339997E-02
506	2.90525115E-02
507	2.93757609E-02
508	2.97038204E-02
509	3.00357640E-02
510	3.03746664E-02
511	3.07176030E-02
512	3.10656539E-02
513	3.14138952E-02
514	3.17774079E-02
515	3.21412733E-02
516	3.25105740E-02
517	3.28853941E-02
518	3.32658192E-02
519	3.36512360E-02
520	3.40439328E-02
521	3.44415994E-02
522	3.48453271E-02
523	3.52551086E-02
524	3.56710382E-02
525	3.60932112E-02
526	3.65217267E-02
527	3.69566821E-02
528	3.73931786E-02
529	3.78463186E-02
530	3.83012063E-02
531	3.87629474E-02
532	3.92316494E-02
533	3.97074217E-02
534	4.01903756E-02
535	4.06806339E-02
536	4.11732817E-02
537	4.16834656E-02
538	4.21952945E-02
539	4.27168393E-02
540	4.32453724E-02
541	4.37818699E-02
542	4.43255055E-02
543	4.48774114E-02
544	4.54407175E-02
545	4.60105575E-02
546	4.65890667E-02
547	4.71763831E-02
548	4.77726462E-02
549	4.83790004E-02
550	4.89925883E-02

TABLE VIII

GOLD

LOWEST ENERGY STATE IS 1.194 RYDBERGS. RADIAL WAVE
FUNCTIONS $R(r)$ AND $\Psi(r)\Psi(r)^*$ WITH r IN 1/100
BOHR UNITS.

R	$\Psi(r)\Psi(r)^*$
551	4.96165592E-02
552	5.02500615E-02
553	5.08932481E-02
554	5.15462738E-02
555	5.22092960E-02
556	5.28824749E-02
557	5.35659733E-02
558	5.42599568E-02
559	5.49645937E-02
560	5.56800552E-02
561	5.64065155E-02
562	5.71441511E-02
563	5.78931425E-02
564	5.86536724E-02
565	5.94259271E-02
566	6.02100259E-02
567	6.10063709E-02
568	6.18149481E-02
569	6.26360264E-02
570	6.34698081E-02
571	6.43164990E-02
572	6.51763085E-02
573	6.60494493E-02
574	6.69361378E-02
575	6.78365942E-02
576	6.87510422E-02
577	6.96797095E-02
578	7.06228276E-02
579	7.15806319E-02
580	7.25533617E-02
581	7.35412606E-02
582	7.45445768E-02
583	7.55635609E-02
584	7.65984693E-02
585	7.76495633E-02
586	7.87171074E-02
587	7.98013710E-02
588	8.09026282E-02
589	8.20211576E-02
590	8.31572427E-02
591	8.43111719E-02
592	8.54832384E-02
593	8.66737403E-02
594	8.78829911E-02
595	8.91112693E-02
596	9.03589185E-02
597	9.16262484E-02
598	9.29135831E-02
599	9.42212530E-02
600	9.55495941E-02

TABLE VIII

GOLD

LOWEST ENERGY STATE IS 1.194 RYDBERGS. RADIAL WAVE
FUNCTIONS $R(r)$ AND $\Psi(r)\Psi(r)^*$ WITH r IN 1/100
BOHR UNITS.

R	$\Psi(r)\Psi(r)^*$
601	9.68989478E-02
602	9.82676610E-02
603	9.96620895E-02
604	1.01076590E-01
605	1.02513530E-01
606	1.03973281E-01
607	1.05456321E-01
608	1.06962735E-01
609	1.08473214E-01
610	1.10048058E-01
611	1.11627671E-01
612	1.13232465E-01
613	1.14862850E-01
614	1.16510220E-01
615	1.18202162E-01
616	1.19911946E-01
617	1.21649090E-01
618	1.23414020E-01
619	1.25207235E-01
620	1.27029194E-01
621	1.28889037E-01
622	1.30761275E-01
623	1.32672385E-01
624	1.34614219E-01
625	1.36587274E-01
626	1.38592092E-01
627	1.40629200E-01
628	1.42699139E-01
629	1.44802463E-01
630	1.46939731E-01
631	1.49111514E-01
632	1.51318394E-01
633	1.53550962E-01
634	1.55839818E-01
635	1.58155574E-01
636	1.60508854E-01
637	1.62900289E-01
638	1.65330524E-01
639	1.67800214E-01
640	1.70310026E-01
641	1.72860640E-01
642	1.75452744E-01
643	1.78087042E-01
644	1.80764247E-01
645	1.83485088E-01
646	1.86250303E-01
647	1.89050647E-01
648	1.91916884E-01
649	1.94819793E-01
650	1.97770169E-01

TABLE VIII

GOLD

LOWEST ENERGY STATE IS 1.194 RYDBERGS. RADIAL WAVE
FUNCTIONS $R(r)$ AND $\Psi(r)\Psi(r)^*$ WITH r IN 1/100
BOHR UNITS.

R	$\Psi(r)\Psi(r)^*$
651	2.00768517E-01
652	2.03816546E-01
653	2.06914177E-01
654	2.10062347E-01
655	2.13262506E-01
656	2.16514919E-01
657	2.19820667E-01
658	2.23130643E-01
659	2.26595760E-01
660	2.30066943E-01
661	2.33595134E-01
662	2.37131290E-01
663	2.40826322E-01
664	2.44553142E-01
665	2.48297403E-01
666	2.52125350E-01
667	2.56016310E-01
668	2.59997134E-01
669	2.63993133E-01
670	2.68077985E-01
671	2.72231806E-01
672	2.76454139E-01
673	2.80746141E-01
674	2.85103929E-01
675	2.89543880E-01
676	2.94052034E-01
677	2.98634690E-01
678	3.03293109E-01
679	3.08029574E-01
680	3.12842390E-01
681	3.17735886E-01
682	3.22710410E-01
683	3.27767340E-01
684	3.32908071E-01
685	3.38134027E-01
686	3.43446655E-01
687	3.48847422E-01
688	3.54337843E-01
689	3.59919420E-01
690	3.65593720E-01
691	3.71362211E-01
692	3.77226801E-01
693	3.83198923E-01
694	3.89270037E-01
695	3.95441213E-01
696	4.01676935E-01
697	4.08045897E-01
698	4.14521072E-01
699	4.21104200E-01
700	4.27797114E-01

TABLE VIII

GOLD

LOWEST ENERGY STATE IS 1.194 RYDBERGS. RADIAL WAVE
FUNCTIONS $R(R)$ AND $\Psi(R)\Psi(R)^*$ WITH R IN 1/100
BOHR UNITS.

R	$\Psi(R)\Psi(R)^*$
701	4.34601689E-01
702	4.41519833E-01
703	4.48553486E-01
704	4.55704623E-01
705	4.62975254E-01
706	4.70357422E-01
707	4.77833208E-01
708	4.85524728E-01
709	4.93304136E-01
710	5.01193623E-01
711	5.09225418E-01
712	5.17301790E-01
713	5.25605047E-01
714	5.34137537E-01
715	5.42721651E-01
716	5.51449820E-01
717	5.60324517E-01
718	5.69348261E-01
719	5.78523614E-01
720	5.87853191E-01
721	5.97339616E-01
722	6.06985617E-01
723	6.16793931E-01
724	6.26767353E-01
725	6.36908724E-01
726	6.47220941E-01
727	6.57706946E-01
728	6.68369736E-01
729	6.79212360E-01
730	6.90237921E-01
731	7.01440573E-01
732	7.12850555E-01
733	7.24444070E-01
734	7.36233507E-01
735	7.48222231E-01
736	7.60413688E-01
737	7.72811392E-01
738	7.85418882E-01
739	7.98239817E-01
740	8.11277885E-01
741	8.24536332E-01
742	8.38020092E-01
743	8.51732789E-01
744	8.65677688E-01
745	8.79859091E-01
746	8.94231051E-01
747	9.08948292E-01
748	9.23864466E-01
749	9.39034095E-01
750	9.54461583E-01

TABLE VIII

GOLD

LOWEST ENERGY STATE IS 1.194 RYDBERGS. RADIAL WAVE
FUNCTIONS $R(r)$ AND $\Psi(r)\Psi(r)^*$ WITH r IN $1/100$
BOHR UNITS.

R	$\Psi(r)\Psi(r)^*$
751	9.70151407E-01
752	9.86108126E-01
753	1.00233638E+00
754	1.01834089E+00
755	1.03562645E+00
756	1.05269797E+00
757	1.07006041E+00
758	1.08771884E+00
759	1.10567842E+00
760	1.12394438E+00
761	1.14252208E+00
762	1.16141693E+00
763	1.18063443E+00
764	1.20018034E+00
765	1.22006025E+00
766	1.240289004E+00
767	1.26084564E+00
768	1.28176309E+00
769	1.30303232E+00
770	1.32467820E+00
771	1.34668830E+00
772	1.36907590E+00
773	1.39184698E+00
774	1.41500846E+00
775	1.43856717E+00
776	1.46253006E+00
777	1.48690421E+00
778	1.51169683E+00
779	1.53691524E+00
780	1.56256690E+00
781	1.58865941E+00
782	1.61520050E+00
783	1.64219804E+00
784	1.66956003E+00
785	1.69739463E+00
786	1.72571013E+00
787	1.75449149E+00
788	1.78431777E+00
789	1.81422724E+00
790	1.84446523E+00
791	1.87556020E+00
792	1.90703566E+00
793	1.93911255E+00
794	1.97169227E+00
795	2.00483455E+00
796	2.03854930E+00
797	2.07234660E+00
798	2.10773671E+00
799	2.14323007E+00
800	2.17933731E+00

TABLE VIII

GOLD

LOWEST ENERGY STATE IS 1.194 RYDBERGS. RADIAL WAVE
FUNCTIONS $R(R)$ AND $\Psi(R)\Psi(R)^*$ WITH R IN 1/100
BOHR UNITS.

R	$\Psi(R)\Psi(R)^*$
801	2.21606924E+00
802	2.25343693E+00
803	2.29145154E+00
804	2.33012449E+00
805	2.36946742E+00
806	2.40949214E+00
807	2.45021070E+00
808	2.49163534E+00
809	2.53377853E+00
810	2.57665303E+00
811	2.62027169E+00
812	2.66464771E+00
813	2.70979446E+00
814	2.75572560E+00
815	2.80245500E+00
816	2.84999680E+00
817	2.89836536E+00
818	2.94757534E+00
819	2.99764165E+00
820	3.04857946E+00
821	3.10040421E+00
822	3.15313163E+00
823	3.20677773E+00
824	3.26135880E+00
825	3.31689143E+00
826	3.37339252E+00
827	3.43087925E+00
828	3.48936913E+00
829	3.54887997E+00
830	3.60942991E+00

APPENDIX IV

FORTRAN COMPUTATIONAL PROGRAMS

THE FOLLOWING PROGRAMS WERE USED IN THE COMPILATION OF DATA AND RESULTS ACHIEVED. THESE PROGRAMS ARE PREPARED IN FORTRAN 50 LANGUAGE FOR THE 1604 CONTROL DATA COMPUTER. THE READER SHOULD KEEP IN MIND THAT THESE PROGRAMS ARE THE END PRODUCTS OF MANY SMALLER PROGRAMS AND BUILT FOR FLEXIBILITY. AS A RESULT SOME OF THE FORTRAN PROGRAMMING MAY NOT BE THE MOST EFFICIENT. THE GRAPH ROUTINE UTILIZED THE CONTROL DATA 160 COMPUTER, CONTROL DATA 165 PLOTTER AND CALIFORNIA COMPUTER PRODUCTS 565 FOR REPRODUCTION.

THE SOLUTION TO THE TRINOMIAL EQUATION FOR SODIUM, CODE NAME BIG ONE, PROCEIVED POTENTIAL. CELLULAR CALCULATION FOR GOLD, CODE NAME BOHR-S, USING THE NEW POTENTIAL IS INDICATED AT PAGES TO IONIZATION ENERGY, SEARCH FOR THE VALUES OF THE PARAMETERS MEETING TO IT IS NOTED THAT THE CELLULAR CALCULATION IS MADE ONCE THE BOUNDARY CONDITIONS ARE SATISFIED.

THE GRAPH ROUTINE FOR THE PLOTTING OF $R(R)$ FROM KNOWN POTENTIALS IS INDICATED AT PAGES TO THE PLOTTING OF $R(R)$, $PSI(R)$ AND $PSI(R)PSI(R)$ * FOR THE NEW POTENTIAL IS INDICATED AT PAGES TO .

..JOB*MUSORRAFITI AND SLAZAK THESIS BIG ONE FEB 1964.

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PROGRAM THESIS
DIMENSION A(670), Y1(667), Y2(667), Y3(667), Y4(667),
1Y6(670), Y7(670), Y8(670), F1(1), F2(1), F3(1), F4(1), F5(1),
2F6(1), F7(1), F8(1), F9(1), F10(1), F11(1), F12(1), F13(1),
3F14(1), F15(1), F16(1), F17(1), F18(1), F19(1), F20(1), F21(1),
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17F123(1), F124(1), F125(1), F126(1), F127(1), F128(1), F129(1),
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57F403(1), F404(1), F405(1), F406(1), F407(1), F408(1), F409(1),
58F410(1), F411(1), F412(1), F413(1), F414(1), F415(1), F416(1),
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83F585(1), F586(1), F587(1), F588(1), F589(1), F590(1), F591(1),
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F4(1)=- (2. *Z*F3(1))-2. *EASY*F2(1))/30.
F5(1)=- (2. *Z*F4(1))-2. *EASY*F3(1))/32.
F6(1)=- (2. *Z*F5(1))-2. *EASY*F4(1))/42.
F7(1)=- (2. *Z*F6(1))-2. *EASY*F5(1))/56.
F8(1)=- (2. *Z*F7(1))-2. *EASY*F6(1))/72.
F9(1)=- (2. *Z*F8(1))-2. *EASY*F7(1))/90.
F10(1)=- (2. *Z*F9(1))-2. *EASY*F8(1))/110.
F11(1)=- (2. *Z*F10(1))-2. *EASY*F9(1))/132.
F12(1)=- (2. *Z*F11(1))-2. *EASY*F10(1))/156.
F13(1)=- (2. *Z*F12(1))-2. *EASY*F11(1))/182.
F14(1)=- (2. *Z*F13(1))-2. *EASY*F12(1))/210.
F15(1)=- (2. *Z*F14(1))-2. *EASY*F13(1))/240.
OY1(1)=H+F1(1)+6. *H*15+16. *F15(1)*H**15
1+F5(1)+F10(1)+H**6+F6(1)+H**15+F15(1)*H**16
2**14+F14(1)*H**15+15. *F15(1)*H**12+F12(1)*H**13+F13(1)*H**
3*14+F14(1)*H**15+15. *F15(1)*H**12+F12(1)*H**13+F13(1)*H**
OY2(1)=1.+2. *H*15+16. *F15(1)*H**15
2*F8(1)+H**4+6. *H*15+16. *F15(1)*H**15
3*H**11+13. *F12(1)*H**12+14. *F13(1)*H**13+15. *F14(1)*H**
4*H**14+H**14+16. *F15(1)*H**15
THE COEFFICIENTS OF THE LOGARITHMIC FUNCTION
X4=I
X1=X4*H-H
X2=X4*H+H
X3=X4*H+H
T1=(X2*(X3**2)-(X3**2)*(X2**2))
T2=(X1*(X3**2)-(X3**2)*(X1**2))
T3=(X1*(X2**2)-(X2**2)*(X1**2))
T4=(X3**2)-(X1**2)
T5=(X3**2)-(X1**2)
T6=X2-X1
T7=X2-X1
T8=X2-X1
T9=T1-T2+T3
P1=A1-(A16)*T1-A(1)*T2+A(11)*T3)/P1
A2=-(A16)*T4-A(1)*T5+A(11)*T6)/P1
A3=(A16)*T7-A(1)*T8+A(11)*T9)/P1
BB(1)=2. *A1*Z
QQ(1)=2. *A2*Z-2. *EASY
RR(1)=2. *Z*A3
DO 200 J=4,75
J6=J-1
J2=J-2
J3=J-3
CO=J

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F(I,1)=-PB(I)/2.
F(I,2)=- (BB(I)*F(I,1)+CC(I))/6.
F(I,3)=- (BB(I)*F(I,2)+CC(I)*F(I,1)+RR(I))/12.
OF(I,J)=- (BB(I)*F(I,J6)+CC(I)*F(I,J2)+RR(I)*F(I,J3))/
1((CO+1.)*CO)
200 CONTINUE
DO 201 J=1,75
CO=J
AA(I,J)=(ON*H-H)**CO
201 CONTINUE
BAD1=0.0
DO 202 J=2,75
J6=J-1
BAD1=AA(I,J)*F(I,J6)+BAD1
202 CONTINUE
REE(I)=CN*H-H+BAD1
DO 203 J=1,75
CO=J
AB(I,J)=(ON*H)**CO
203 CONTINUE
ADD1=0.0
DO 204 J=2,75
J6=J-1
ADD1=AB(I,J)*F(I,J6)+ADD1
204 CONTINUE
STAY(I)=ADD1+ON*H
ADD2=0.0
DO 205 J=2,75
CO=J
ADD2=(CO+1.)*F(I,J)*AB(I,J) +ADD2
205 CONTINUE
PLAY(I)=1.+2.*F(I,1)*ON*H+ADD2
ADD3=0.0
DO 206 J=2,75
CO=J
ADD3=(CO+1.)*(F(I,J)*AA(I,J))+ADD3
206 CONTINUE
SEE(I)=1.+2.*F(I,1)*(ON*H-H)+ADD3
POT(I)=LOGF(ON-1.)/H
ROT(I)=LOGF(CN)-LOGF(1./H)
V(I,1)=-BB(I)
VV(I,1)=PB(I)
AC(I,1)=-RR(I)
PC(I,1)=PB(I)
G(I,1)=-PB(I)*POT(I)+PB(I)
S(I,1)=-BB(I)*BOT(I)+BB(I)
V(I,2)=-BB(I)*AC(I,1)/2.

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W(I,1)=0.0
WW(I,2)=-QQ(I)/2.
VV(I,2)=-BB(I)*(BC(I,1)/2.-AC(I,1)*3./4.)
AC(I,2)=VV(I,2)+WW(I,2)
BC(I,2)=AC(I,2)*POT(I)+BC(I,2)
G(I,2)=AC(I,2)*BOT(I)+BC(I,2)
S(I,2)=AC(I,2)*AC(I,2)/6.
W(I,3)=-QQ(I)*AC(I,1)/6.
VV(I,3)=-BB(I)*(-AC(I,2)*5./36.+BC(I,2)/6.)
WW(I,3)=-QQ(I)*(-AC(I,1)*5./36.+BC(I,1)/6.)
XX(I,3)=-RR(I)/6.
AC(I,3)=VV(I,3)+W(I,3)+XX(I,3)
BC(I,3)=VV(I,3)+WW(I,3)+BC(I,3)
G(I,3)=AC(I,3)*POT(I)+BC(I,3)
S(I,3)=AC(I,3)*BOT(I)+BC(I,3)
CAL(1)=(BB(I)+AC(I,1))/ON*F
CAL(2)=BB(I)*S(I,1)+QQ(I)+2.*S(I,2)+3.*AC(I,2)
OCAL(3)=BB(I)*S(I,2)+QQ(I)*S(I,1)+6.*S(I,3)+5.*
1AC(I,3)
DO 256 J=4,75
CO=J
J2=J-2
J3=J-3
OVV(I,J)=-BB(I)*(-AC(I,J6)*(2.*CO-1.)/(CO*(CO-1.))**2
1+BC(I,J6)/(CO*(CO-1.)))
OWW(I,J)=-QQ(I)*(-AC(I,J2)*(2.*CO-1.)/(CO*(CO-1.))**2
1+BC(I,J2)/(CO*(CO-1.)))
OXX(I,J)=-RR(I)*(-AC(I,J3)*(2.*CO-1.)/(CO*(CO-1.))**2
1+BC(I,J3)/(CO*(CO-1.)))
AC(I,J)=V(I,J)+W(I,J)+X(I,J)
RC(I,J)=VV(I,J)+WW(I,J)+XX(I,J)
G(I,J)=AC(I,J)*POT(I)+BC(I,J)
S(I,J)=BC(I,J)+BOT(I)*AC(I,J)
OCAL(J)=RH(I)*S(I,J6)+QQ(I)*S(I,J2)+RR(I)*S(I,J3)+
1CO*(CO-1.)*S(I,J)+(2.*CO-1.)*AC(I,J)
256 CONTINUE
ADD4=0.0
DO 207 J=1,75
ADD4=G(I,J)*AA(I,J)+ADD4
207 CONTINUE
BUM(I)=1.+ADD4
ADD6=0.0
DO 209 J=2,75
J6=J-1
CO=J
ADD6=AA(I,J6)*(CO*G(I,J)+AC(I,J))+ADD6

```



```

209 CONTINUE
CUM(I)=G(I,1)+AC(I,1)+ACD6
ADD5=0.0
DO 208 J=1,75
ADD5=S(I,J)*AB(I,J)+ADD5
208 CONTINUE
DRAY(I)=1.+ADD5
ADD7=0.0
DO 210 J=2,75
J6=J-1
CO=J
ADD7=AB(I,J6)*(CO*S(I,J)+AC(I,J))+ADD7
210 CONTINUE
BRAY(I)=S(I,1)+AC(I,1)+ADD7
ADD8=0.0
DO 211 J=2,75
CO=J
J6=J-1
ADD8=CO*(CO+1.)*F(I,J)*AB(I,J6)+ADD8
211 CONTINUE
TEE(I)=2.*F(I,1)+ADD8
ADD9=0.0
DO 212 J=3,75
J2=J-2
CO=J
OADD9=AB(I,J2)*(CO*(CO-1.)*S(I,J)+(2.*CO-1.)*AC(I,J))+
1ADD9
212 CONTINUE
TUM(I)=AC(I,1)/(ON*H)+2.*S(I,2)+3.*AC(I,2)+ADD9
DOPE(I)=(RUM(I)*SEE(I)-CUM(I)*BEE(I))
ABLE(I)=(Y1(I6)*SEE(I)-Y2(I6)*BEE(I))/DOPE(I)
BOZC(I)=(Y2(I6)*BUM(I)-Y1(I6)*CUM(I))/DOPE(I)
AK1=ON*H
Y1(I)=ABLE(I)*DRAY(I)+BOZC(I)*STAY(I)
Y2(I)=ABLE(I)*BRAY(I)+BOZO(I)*PLAY(I)
Y3(I)=Y1(I)/AK1
Y4(I)=Y3(I)-Y2(I)
Y6(I)=ABLE(I)*TUM(I)+BOZO(I)*TEE(I)
Y7(I)=-2.*(Z*A(I)/(ON*H)-EASY)*Y1(I)
PRINT 884,I
HION=.372
CE(I)=(-2.*EASY+2.2/(AK1**2)+HION)*310.5
20 CONTINUE
LADL=(4HNO=1)
CALL GRAPH2(667,XYZ,Y1,8,1,LABEL,ITITLE,0,0,0,0,0,0,0)
LABEL=(4HNO=2)

```



```

CALL GRAPH2(667,XYZ,Y2,8,2,LABEL,ITITLE,0,0,0,0,0,0,0)
LABEL=(4HNO=3)
CALL GRAPH2(667,XYZ,Y3,8,3,LABEL,ITITLE,0,0,0,0,0,0,0)
EASY=0.1
IF(EASY-.35)10,555,555

```

```

555 END

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...JOB*SLAZAK AND MUSORRAFITI BOX 71 BOHR S
PROGRAM THESIS
DIMENSION Y1(600), Y2(674), Y3(674), Y4(674), R(674), R1(6
174), CE(674), A(674), Y6(674), Y7(674), F1(1), F2(1), F3(1),
2F4(1), F5(1), F6(1), F7(1), F8(1), F9(1), F10(1), F11(1), F12
3(1), F13(1), F14(1), F15(1), X(600), ITITLE(10), R2(667)
DO 1234 I=1, 10
1234 ITITLE(I)=(8H SLAZAK )
ITITLE(1)=(8H SLAZAK )
ITITLE(2)=(8H AND MUSO)
ITITLE(3)=(8H RRAFITI )
ITITLE(4)=(8H BOX 71 )
ITITLE(5)=(8H GOLD )
DO 999 I=1, 600
999 X(I)=I
Z=79.
PRINT 60
600 FORMAT(10H1 RYDBERGS N 20H 20H BOHR 3AD11 20H RYDBERGS
1 20H RYDBERGS 24H COHESIVE KCAL P
2ER MOLE /// )
HICN=.666
EASY=.500
SY=.875
SX=.0826
ST=1.429
2 9 DO 604 J=1, 300
ZN=J
H=.01
AK=ZN*H
OSU=(1./LOGF(3.))*(LOGF(LOGF((1.-SX)*COSF(3.*SY)/(1.021-SX))) )
1-LOGF(ST))
A(J)=(1.-SX)*COSF(SY*AK)/EXPF(ST*AK**SU)+SX
604 CONTINUE
DO 605 J=301, 600
ZN=J
H=.01
AK=ZN*H
A(J)=.105/(AK+2.)
605 CONTINUE
H=.01
B=2.*Z
Q=2.*Z*(4.*(A(2)-1.)-2.*(A(3)-1.))/2.*H -2.*EASY
R=2.*Z*(A(3)-2.*(A(2)+1.))/(2.*H*H)
F1=-B/2
F2=-B*F1/2 -Q/6.
F3=-(B*F2-Q*F1-R)/12.
F4=-(B*F3-Q*F2-R*F1)/20.

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F5=- (B *F4 -Q *F3 -R *F2)/30.
F6=- (B*F5 -Q*F4 -R*F3)/42.
F7=- (B*F6 -Q*F5 -R*F4)/56.
F8=- (B*F7 -Q*F6 -R*F5)/72.
F9=- (B*F8 -Q*F7 -R*F6)/90.
F10=- (B*F9 -Q*F8 -R*F7)/110.
H=.01
SK=2.*H
OY1(I)=H+F1*H*H +F2*H**3 +F3*H**4+F4*H**5 +F5*H**6
1+F6*H**7+F7*H**8+F8*H**9 + F9*H**10+F10*H**11
OY1(2)=SK+F1*SK**2+F2*SK**3 + F3*SK**4+F4*SK**5
1+F5*SK**6+F6*SK**7+F7*SK**8 +F8*SK**9+F9*SK**10
2+F10*SK**11
Y1(3)=Y1(2)* (2.-H*H*2.*(Z*A(2)/(H*2.))-EASY))-Y1(1)
Y1(4)=Y1(3)* (2.-H*H*2.*(Z*A(3)/(H*3.))-EASY))-Y1(2)
Y1(5)=Y1(4)* (2.-H*H*2.*(Z*A(4)/(H*4.))-EASY))-Y1(3)
Y1(6)=Y1(5)* (2.-H*H*2.*(Z*A(5)/(H*5.))-EASY))-Y1(4)
DO 12 I=2,599
I1=I+1
I6=I-1
BO=I
ON=I1
Y1(I1)= Y1(I)*(2.-H*H*2.*(Z*A(I)/(H*BO)-EASY))-Y1(I6)
12 CONTINUE
K11=595
DO 30 J=6,K11
J1=J+1
BO=J
J6=J-1
ON=J1
J2=J+2
J3=J+3
J4=J+4
J5=J+5
J11=J-1
J22=J-2
J33=J-3
HJ=J1
HAL3=(Y1(J2)- Y1(J))*4./(5.*H)-(Y1(J3)-Y1(J1))/(5.*H)
OHAL4=(Y1(J4)- Y1(J22))*4./(105.*H)-(Y1(J5)-Y1(J33))/
1 (280.*H)
Y2(J1)=HAL3+HAL4
Y3(J1)=Y1(J1)/(H*ON)
Y4(J1)=Y3(J1)-Y2(J1)
AP=ABSF(Y4(J1))
IF (AB-1.E-3)13,13,30
13 R(J1)=-2.*EASY+2.2/((H*CN)*(H*ON))

```



```

R1(J1)=R(J1)+HION
R2(J1)=2.*EASY
CE(J1)=R1(J1)*310.5
PRINT 221,J1,R2(J1),R(J1),Y4(J1),CE(J1)
221 FORMAT(I10,1P5E20.8)
30 CONTINUE
EASY=EASY+.005
IF(EASY-.600)2,2,556
556 END
END

```



```

..JOB*SLAZAK AND MUSORRAFITI BOX 71 SEARCH
PROGRAM THESIS
DIMENSION Y1(830),Y2(830),Y3(674),Y4(830),R(674),R1(674),CE(674),
1A(830),Y6(674),Y7(674),F1(1),F2(1),F3(1),F4(1),F5(1),F6(1),
2F7(1),F8(1),F9(1),F10(1),F11(1),F12(1),F13(1),F14(1),F15(1),
3 R2(667),O(830),OO(830)
DO 999 I=1,600
999 X(I)=1
PRINT 60
600 FORMAT(10H1,RYDBERGS N 20H 20H BOHR RAD11 20H RYDBERGS
1 20H RYDBERGS 24H COHESIVE KCAL P
2ER MCLE ///)
Z=79.
EASY=.333
ST=1.250
SX=.047
SY=.875
SB=3.0
SZ=LOGF((COSF(SY*SB))*(1.-SX)/(3.5369/Z-SX))
SU=LOGF(SZ/ST)/LCGF(3.0)
SG=3.0
SE=.021
SB=20.0
SU1=(SE/((SB+SG)*(SE-SX))-SY*TANF(SY*SG))*(1./SZ)
SA=SG*SZ/(SG**SU1)
SD=SA-ST
PRINT 525,SU1,SA,SD
525 9 FORMAT(1P3E20.8)
DO 604 J=1,300
ZN=J
H=.01
AK=ZN*H
A(J)=(1.-SX)*COSF(SY*AK)/EXPF(ST*AK**SU)+SX
604 CONTINUE
DO 605 J=301,830
TT=(3.+SB)*SE/(AK+SB)
TK=1./Z
IF(TT-TK)811,811,812
811 A(J)=TK
GO TO 605
812 A(J)=TT
605 CONTINUE
H=.01
B=2.*Z
Q=2.*Z*(4.*(A(2)-1.)-2.*(A(3)-1.))/2.*H -2.*EASY
R=2.*Z*(A(3)-2.*A(2)+1.)/(2.*H*H)
F1=-B/2.

```



```

F2=-B*F1/2.-Q/6.-Q*F1-R)/12.-R*F1)*F2)/20./30.
F3=-(B*F2-Q*F2-Q*F3-R*F3)*F2)/30.
F4=-(B*F3-Q*F3-Q*F4-R*F4)*F3)/42.
F5=-(B*F4-Q*F4-Q*F5-R*F5)*F4)/56.
F6=-(B*F5-Q*F5-Q*F6-R*F6)*F5)/72.
F7=-(B*F6-Q*F6-Q*F7-R*F7)*F6)/90.
F8=-(B*F7-Q*F7-Q*F8-R*F8)*F7)/110.
F9=-(B*F8-Q*F8-Q*F9-R*F9)*F8)/130.
H=.01
SK=2.*H
OY1(1)=H+F1*H*H+F2*H*H*3+F3*H*H*4+F4*H*H*5+F5*H*H*6
OY1(2)=H+F6*H*H*7+F7*H*H*8+F8*H*H*9+F9*H*H*10+F10*H*H*11
OY1(3)=SK+F1*SK**2+F2*SK**3+F3*SK**4+F4*SK**5
OY1(4)=SK**6+F5*SK**7+F6*SK**8+F7*SK**9+F8*SK**10
OY1(5)=SK**11
DO 12 I=2,829
I1=I+1
I6=I-1
BO=I
ON=I1
Y1(I1)=Y1(I)*(2.-H*H*2.*(Z*A(I))/(H*BO)-EASY))-Y1(I6)
12 CONTINUE
AB=Y1(820)
PRINT 557,AB
PRFORMAT(1P6,E20.8)
PRFORMAT(1P6,E20.8)
PRFORMAT(1P5,E20.8)
IF(AB-1.E-3)23,223,223
ST=ST+.005
AQ=ABSF(SD)
IF(ST-1.940)3,3,22
IF(SD-1.E-3)223,323,242
IF(AQ-1.E-3)323,323,225
IF(AQ-1.E-3)323,323,225
SX=ST-.001
ST=ST-.025
GO TO 3
HION=.666
EASY=.500
K33=1
H=.01
DO 191 L=1,K33
R=2.*Z
O=2.*Z*(4.*(A(2)-1.)-2.*(A(3)-1.))/2.*H-2.*EASY
R=2.*Z*(A(3)-2.*A(2)+1.)/(2.*H*H)
F1=-R/2.

```



```

13 IF (AB-1.E-3) 13, 13, 32
   R(J1)=-2.*EASY+2.2/((H*CN)*(H*ON))
   R2(J1)=R(J1)+HION
   R2(J1)=2.*EASY
   CE(J1)=R1(J1)*310.5
   PRINT 221, J1, R2(J1), R(J1), Y4(J1), CE(J1)
   FORMAT(I10, 1P5E20.8)
221 CONTINUE
32 EASY=EASY+.005
   IF (EASY-.75) 52, 52, 191
191 GO TO 556
22 SX=SX+.001
   ST=ST-.025
   IF (SX-.095) 3, 3, 556
556 END
END

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..JOB*MUSORRAFITI AND SLAZAK          BOX 71      FERMI-GOLD
PROGRAM THIS IS
THOMAS-FERMI, HARTREE AND HARTREE-FOCH POTENTIALS
WERE USED IN LIKE PROGRAMS TO MAKE SIMILIAR
CALCULATIONS AND THE VALUES OBTAINED COMPARED WITH
THOSE OBTAINED FROM THE SLAZAK-MUSORRAFITI POTENTIAL.
DIMENSION Y1(830), Y2(674), Y3(674), Y4(674), R(674),
IR1(674), CE(674), A(830), Y6(674), Y7(674), X(830), ITITLE(
210), R2(674)
DO 1234 I=1, 10
ITITLE(I)=(8H SLAZAK )
ITITLE(I)=(8H SLAZAK )
ITITLE(2)=(8H HAND MUSO)
ITITLE(3)=(8H RRAFITI )
ITITLE(4)=(8H BOX 71 )
ITITLE(5)=(8H FERMI )
ITITLE(6)=(8H GOLD )
READ 223, (A(I), I=1, 610)
DO 998 I=611, 830
A(I)=A(610)
223 FORMAT(5F10.0)
999 DO 999 I=1, 830
X(I)=I
CALL GRAPH2(830, X, A , 8, 0, 0, ITITLE, 0, 0, 0, 0, 0, 0)
Z=79.
HICON=.280
EASY=.18
2 H=.01
R=2.*Z*(4.*(A(2)-1.)-2.*(A(3)-1.))/2.*H -2.*EASY
Q=2.*Z*(A(3)-2.*A(2)+1.)/(2.*H*H)
R1=-B/2.
F1=-R*F1/2. -Q/6.
F2=-R*F2-Q*F1-R)/12.
F3=-R*F3-Q*F2-Q*F1-R)/20.
F4=-R*F4-Q*F3-Q*F2-Q*F1-R)/30.
F5=-R*F5-Q*F4-Q*F3-Q*F2-Q*F1-R)/42.
F6=-R*F6-Q*F5-Q*F4-Q*F3-Q*F2-Q*F1-R)/56.
F7=-R*F7-Q*F6-Q*F5-Q*F4-Q*F3-Q*F2-Q*F1-R)/72.
F8=-R*F8-Q*F7-Q*F6-Q*F5-Q*F4-Q*F3-Q*F2-Q*F1-R)/90.
F9=-R*F9-Q*F8-Q*F7-Q*F6-Q*F5-Q*F4-Q*F3-Q*F2-Q*F1-R)/110.
H=.01
SK=2.*H
OY1(1)=H+F1*H**2+F2*H**3+F3*H**4+F4*H**5+F5*H**6
1+F6*H**7+F7*H**8+F8*H**9+F9*H**10+F10*H**11
OY1(2)=SK+F1*SK**2+F2*SK**3+F3*SK**4+F4*SK**5
1+F5*SK**6+F6*SK**7+F7*SK**8+F8*SK**9+F9*SK**10

```



```

2+FL0*SK**11
Y1(3)=Y1(2)* (2.-H*H*2.*(Z*A(2)/(H*2.)-(EASY))-Y1(1))
Y1(4)=Y1(3)* (2.-H*H*2.*(Z*A(3)/(H*3.)-(EASY))-Y1(2))
Y1(5)=Y1(4)* (2.-H*H*2.*(Z*A(4)/(H*4.)-(EASY))-Y1(3))
Y1(6)=Y1(5)* (2.-H*H*2.*(Z*A(5)/(H*5.)-(EASY))-Y1(4))
DO 12 I=2,829
  I1=I+1
  I6=I-1
  BO=I1
  ON=I1
  Y1(I1)= Y1(I)*(2.-H*H*2.*(Z*A(I)/(H*BO)-EASY))-Y1(I6)
12 CONTINUE
CALL GRAPH2(830,X,Y1,8,C,0,ITITLE,C,0,0,0,0,0,0)
EASY=EASY+.01
IF(EASY-.22)2,2,556
END
END

```

12

556

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9542 7620
.7290 .6180
.5950 .5140
.4980 .4350
.4200 .3750
.3660 .3260
.3160 .2860
.2790 .2525
.2470 .2215
.220 1838
.1975 1490
.1775 1360
.1605 1150
.1463 1067
.1325 982
.1235 901
.1135 825
.1051 770
.0882 718
.0814 672
.0759 631
.0664 594
.0625 560
.0587 530
.0554 505
.0524 473
.0495 439

8000 8000
.6320 .5320
.4320 .3870
.3320 .3260
.2920 .2600
.2315 .2060
.206 1650
.1850 1518
.1575 1375
.1375 1270
.1170 1082
.1082 1000
.0918 918
.0838 838
.0780 780
.0729 729
.0681 681
.0639 639
.0601 601
.0566 566
.0536 536
.0506 506
.0479 479

8400 8400
.6680 .5520
.4680 .3980
.3450 .3000
.2660 .236
.211 188
.1708 154
.154 141
.141 129
.129 119
.119 110
.1018 934
.0852 852
.0791 791
.0739 739
.0690 690
.0647 647
.0609 609
.0573 573
.0542 542
.0512 512
.0484 484

8920 8920
.6990 .5730
.4800 .4090
.3550 .3090
.2720 .2420
.216 192
.1748 152
.1575 145
.1445 131
.1321 121
.119 113
.1035 103
.0862 862
.0802 802
.0749 749
.0695 695
.0655 655
.0617 617
.0580 580
.0548 548
.0518 518
.0489 489

```



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..JOB*SLAZAK AND MUSORRAFITI      GOLD
PROGRAM THESIS
DIMENSION Y1(830), Y2(830), Y3(674), Y4(830), R(674),
1R1(674), CE(674), A(830), Y6(674), Y7(574), R2(667), X(830),
2PSI(830), PSI2(830), PSIA(800), PSI2A(800), X1(800),
3ITITLE(10)
DO 1234 I=1,10
1234 ITITLE(I)=(8H SLAZAK )
ITITLE(1)=(8H SLAZAK )
ITITLE(2)=(8H HAND MUSO)
ITITLE(3)=(8HRRAFITI )
ITITLE(4)=(8HBCX 71 )
ITITLE(5)=(8HOUR )
ITITLE(6)=(8HGOLD )
Z=79.
2 ST=1.429
7 EASY=.597
SX=.0826
SG=2.99
SE=.020
K=299
K1=K+1
3 SY=.875
SB=(6.524676
SU=.524676
9 DO 604 J=1,K
ZN=J
H=.01
AK=ZN*H
A(J)=(1.-SX)*COSF(SY*AK)/EXPF(ST*AK**SU)+SX
CONTINUE
DO 605 J=K1,830
ZN=J
H=.01
AK=ZN*H
IT=(SG+SB)*SE/(AK+SB)
TK=1./Z
IF(TT-TK)811,811,812
811 A(J)=TK
GO TO 605
812 A(J)=TT
605 CONTINUE
13 H=.01
R=2.*Z
R=2.*Z*(4.*(A(2)-1.)-2.*(A(3)-1.))/2.*H -2.*EASY
R=2.*Z*(A(3)-2.*(A(2)+1.)/(2.*H*H)
F1=-8/2.

```



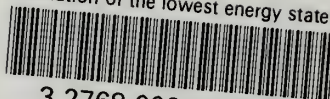
```

F2=-B*F1/2.-Q/6.-Q*F1-R)/12.*F1)/20.*F2)/30.
F3=-B*F2-Q*F2-R*F3-F3)/42.
F4=-B*F3-Q*F3-R*F4-F4)/56.
F5=-B*F4-Q*F4-R*F5-F5)/72.
F6=-B*F5-Q*F5-R*F6-F6)/90.
F7=-B*F6-Q*F6-R*F7-F7)/110.
F8=-B*F7-Q*F7-R*F8-F8)/130.
F9=-B*F8-Q*F8-R*F9-F9)/150.
H=.01
SK=2.*H
OY1(1)=H+F1*H*H+F2*H*H*3+F3*H*H*4+F4*H*H*5+F5*H*H*6
OY1(2)=SK+F1*SK*8+F2*SK*9+F3*SK*10+F4*SK*11
OY1(3)=SK+F1*SK*2+F2*SK*3+F3*SK*4+F4*SK*5
OY1(4)=SK+F1*SK*6+F2*SK*7+F3*SK*8+F4*SK*9+F5*SK*10
DO 12 I=1,829
I1=I+1
I6=I-1
BO=I1
ON=I1
Y1(I1)=Y1(I)*(2.-H*H*2.*(Z*A(I)/(H*BO)-EASY))-Y1(I6)
12 CONTINUE
DO 998 I=1,830
X(I)=I
H=.01
ZN=I
AK=ZN*H
PSI(I)=Y1(I)/AK
PSI2(I)=PSI(I)*PSI(I)
998 CONTINUE
N=1
DO 901 I=30,830
PSIA(N)=PSI(I)
PSI2A(N)=PSI2(I)
XI(N)=X(I)
N=N+1
901 CONTINUE
556 END

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Calculation of the lowest energy state o



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